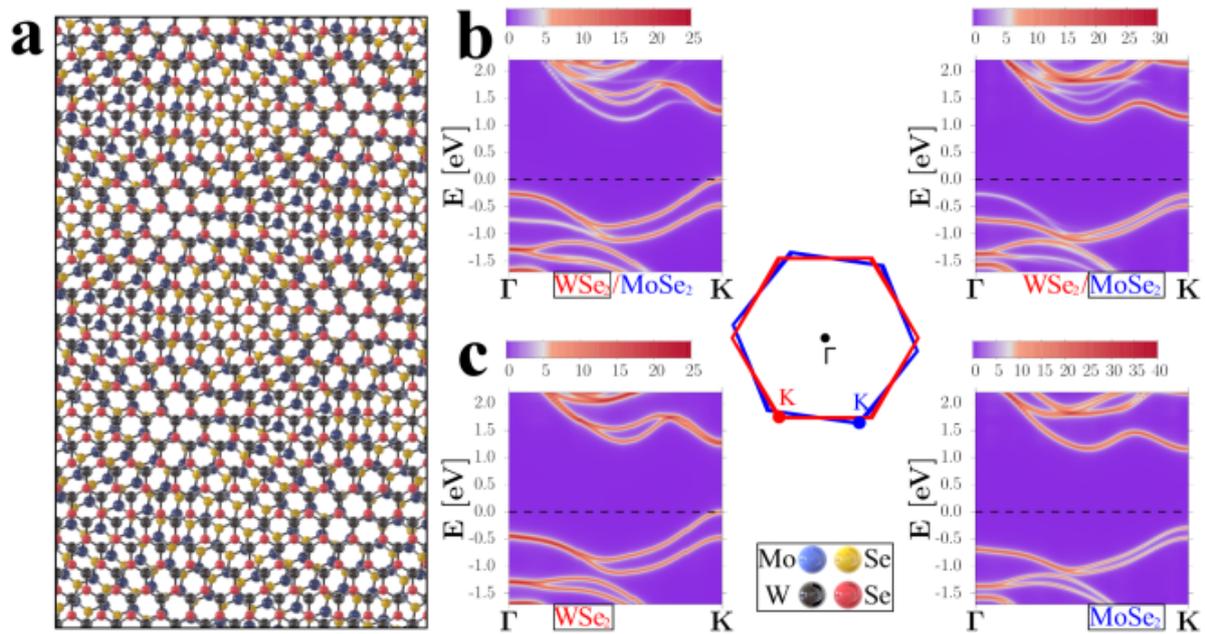


**IOP** | Institute of Physics  
**Computational Physics Group**

Newsletter



Large-scale density functional theory study of van-der-Waals heterostructures  
 (image courtesy of Dr. Gabriel Constantinescu)

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## This Newsletter...

Dear Readers,

The feature article for this bumper edition of the newsletter is an invited contribution by Dr Gabriel Constantinescu from the Cavendish Laboratory, University of Cambridge, UK, the winner of the 2018 IoP Computational Physics Group PhD Prize, on 'Large-scale density functional theory study of van-der-Waals heterostructures'.

Dr Gabriel Constantinescu also kindly provided the cover image for this edition.

Most URLs in the newsletter have web hyperlinks and clicking on them should take you to the corresponding page.

The current edition of the newsletter can be found online at:

[www.iop.org/activity/groups/subject/comp/news/page\\_40572.html](http://www.iop.org/activity/groups/subject/comp/news/page_40572.html)

with previous editions at:

[www.iop.org/activity/groups/subject/comp/news/archive/page\\_53142.html](http://www.iop.org/activity/groups/subject/comp/news/archive/page_53142.html)

The IoP CPG are also pleased to announce the creation of a new group blog, which can be accessed online at [compphysics.org](http://compphysics.org). We would advise you to subscribe to the blog for up-to-date information about events and news items. The subscribe to the blog to follow any updates the reader should press the 'follow' button at the bottom of the page. Suggestions for posts can be send via the blogs contact page, [compphysics.org/contact](http://compphysics.org/contact).

We want to pay tribute to Marco past editor of the newsletter who now has assumed the position of Chair of CPG for work done to date in ensuring the community has been kept up to date on happenings in the group and in the field. The current and future editions will ensure that news of developments in computational physics are reported with signpost provided for increased networking activities in this and allied fields.

Enjoy this edition!

James Uhomoi bhi, Newsletter Editor ✉ [j.uhomoi bhi@ulster.ac.uk](mailto:j.uhomoi bhi@ulster.ac.uk)  
(on behalf of the The Computational Physics Group Committee).

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Some useful web links related to the Computational Physics Group are:

- CPG webpages  
[comp.iop.org](http://comp.iop.org)
- CPG Newsletters Current issue:  
[www.iop.org/activity/groups/subject/comp/news/page\\_40572.html](http://www.iop.org/activity/groups/subject/comp/news/page_40572.html)  
Previous issues:  
[www.iop.org/activity/groups/subject/comp/news/archive/page\\_53142.html](http://www.iop.org/activity/groups/subject/comp/news/archive/page_53142.html)  
[www.soton.ac.uk/~fangohr/iop\\_cpg.html](http://www.soton.ac.uk/~fangohr/iop_cpg.html)

## Related Newsletters and Useful Websites

The Computational Physics Group works together with other UK and overseas computational physics groups. We list their newsletter locations and other useful websites here:

- Newsletter of the Computational Physics Division of the American Physical Society:  
[www.aps.org/units/dcomp/newsletters/index.cfm](http://www.aps.org/units/dcomp/newsletters/index.cfm)
- Europhysicsnews newsletter of the European Physical Society (EPS):  
[www.europhysicsnews.org/](http://www.europhysicsnews.org/)
- Newsletter of the Psi-k ( $\Psi_k$ ) network:  
[www.psi-k.org/newsletters.shtml](http://www.psi-k.org/newsletters.shtml)
- Computational Physics Group blog (CPG):  
[compphysics.org](http://compphysics.org)

# Large-scale density functional theory study of van-der-Waals heterostructures

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## Abstract

Research on two-dimensional (2D) materials currently occupies a sizeable fraction of the materials science community, leading to a comprehensive body of knowledge on such layered structures. We aim to deepen the understanding of the comparatively unknown heterostructures composed of different stacked layers. First, we utilise linear-scaling density functional theory (LS-DFT) to simulate interfaces between promising layered materials, such as transition metal dichalcogenides (TMDC) or black phosphorus (BP) and hexagonal boron nitride (hBN). We show that hBN can protect BP from external influences, prevent band-gap reduction in BP stacks, and enable the use of BP heterostructures as tunnelling field effect transistors. Moreover, we simulate the electronic structure of TMDC interfaces to explain photoemission spectroscopy observations of commensurate and incommensurate phases within the same crystal. Secondly, we have developed a linear-response phonon formalism for LS-DFT, to be used in future studies on 2D heterostructures.

## Introduction

Graphene instantly impressed the scientific community with its enormous electron mobility, but its lack of a band gap eventually paved the way for semiconducting layered materials, notable being transition metal dichalcogenides (TMDCs [1]) such as  $\text{MoS}_2$ ,  $\text{MoSe}_2$ , and  $\text{WSe}_2$ . TMDCs soon demonstrated their value in semiconductor electronics [2], spintronics[3], and optoelectronics[4], but they were hindered by the presence of direct band gaps only in monolayers, and carrier mobilities far smaller than those encountered in graphene. Consequently, the spotlight has recently been shared with black phosphorus (BP), which rectifies the shortcomings of TMDCs through higher carrier mobilities, and a direct band gap that decreases with thickness and covers the electromagnetic spectrum unharnessed by graphene and TMDCs. Unfortunately, BP is highly sensitive to environmental contaminants, and the aforementioned band gap decrease leaves the near-infrared spectrum accessible only to the monolayer. Lastly, the current on/off ratio for BP transistors is low, making BP channels less desirable than TMDC ones.

Consequently, we first show that monolayers of hexagonal boron nitride (hBN) can alleviate the shortcomings of pristine BP. As means of investigation, we utilise the ONETEP [5] linear-scaling density-functional theory (LS-DFT) code to simulate large rotated hBN/BP interfaces. We continue with the account of bandstructure effects that occur when stacking different TMDC layers, in conjunction with angular resolved photoemission spectroscopy (ARPES) performed by experimental collaborators. Simulations of extended heterostructures such  $\text{MoSe}_2/\text{WSe}_2$  agree well with experimentally observed band hybridisations and offsets in TMDC interfaces.

Lastly, we briefly describe a novel linear-scaling implementation of linear-response phonons in the ONETEP code, which serves as a stepping stone for the long-term goal of large-scale Raman spectra calculations. This technique has become a multi-purpose investigation tool for layered materials [6], but existing implementations are impractical for simulating interfaces as large as the ones in our work. The novelty is in developing a new routine for first-order wavefunctions adapted to the particularities of a linear-scaling framework.

## Two-dimensional heterostructures

### hBN/BP

In studying the interfacing of semiconducting black phosphorus (BP) with insulating hexagonal boron nitride (hBN), our test systems were large rotated hBN/BP/hBN and BP/hBN/BP trilayers (Fig. 1), containing 1824 and 1632 atoms

respectively. As a measure of alterations to the electronic band structure we have utilised the one-particle Kohn-Sham spectral function  $A_{k,j,k}(\omega)$ , which is the probability that an electron of momentum  $k$  can be added/removed into/from band  $j$  with an energy  $\omega$ . The work presented here has been published in Nano Letters [7].

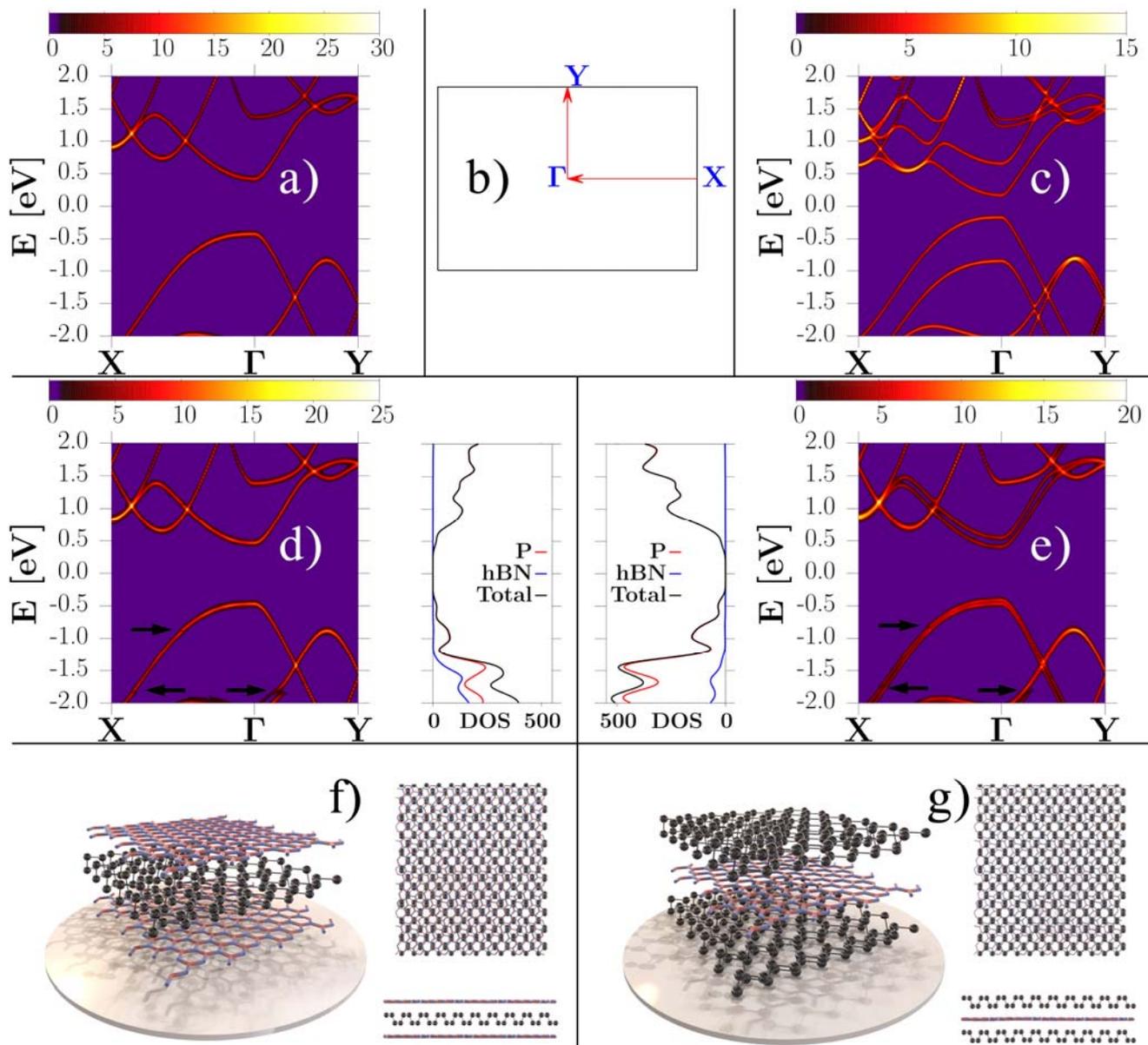


Figure 1: Unfolded spectral function for the BP monolayer (a), the top BP sheet in the BP bilayer (c), the BP layer in the hBN/BP/hBN interface (d), and the top BP sheet in BP/hBN/BP (e). Brillouin-zone sampling path depicted in (b). Black arrows in (d),(e) highlight band discontinuities due to hBN-BP interactions. Schematic representation of hBN/BP/hBN (f) and BP/hBN/BP (g), P atoms are black spheres.

It is experimentally known [8] that hBN substrates shield from unwanted scattering potentials. Comparing the electronic structures of the independent BP monolayer (Fig. 1.a) with the BP sheet in hBN/BP/hBN (Fig. 1.d), it is clear that no alterations have occurred to the DFT-predicted direct band gap (0.84 eV), nor the shape of the bands near the Fermi level. Therefore, hBN-encapsulation produces no undesired effects to the electronic structure of BP, while still protecting from environmental influences [9].

Secondly, we have shown that hBN spacers (i.e. BP/hBN/BP interfaces in Fig. 1.g) counteract band-gap diminishing

in multi-stacked BP sheets[10], such as the observed reduction from a 0.84 eV gap in monolayer BP (Fig. 1.a) to 0.34 eV in the bilayer (Fig. 1.c). We have thus compared the spectral functions between the top BP sheets from the bilayer (Fig. 1.c) and BP/hBN/BP interface (Fig. 1.e). Therefore, the interaction between the wavefunctions of the semiconducting films in BP/hBN/BP is diminished by the hBN spacer, as one reverts to the monolayer bandstructure of BP, with the band gap of the interface increasing to 0.82 eV from 0.34 eV in the bilayer.

The BP/hBN/BP interface is also a candidate for Tunnelling Field Effect Transistor (TFET) architectures, allowing us to perform large-scale device simulations. As in Fig. 2.a, BP/hBN/BP is placed between 4-layer hBN dielectrics and graphene gates on each side, while gate voltages ( $V_{BG}$ ,  $V_{TG}$ ) control the carrier concentrations, and a bias voltage ( $V_{DS}$ ) is maintained between the BP layers.

TMDC channels are preferred in conventional Metal-Oxide-Semiconductor Field Effect Transistors (MOSFETs), as the smaller band gap of BP causes modest on/off current ratios [11, 12], due to thermal excitations inducing interlayer electron injection in the off-state. However, in a TFET arrangement (Fig. 2.a) the hBN barrier inhibits thermal carrier injection, leaving only quantum tunnelling as a current-generation mechanism. We calculate the tunnelling current in the Bardeen formalism [13]:

$$I = \frac{4\pi e}{\hbar} \sum_{i,j} \sum_{\mathbf{k}_B, \mathbf{k}_T} |O_{ij}(\mathbf{K}_B, \mathbf{K}_T)|^2 \delta[E_{iB}(\mathbf{K}_B) - E_{jT}(\mathbf{K}_T)] (f_{iB} - f_{jT}), \quad (1)$$

where  $\mathbf{k}$ ,  $E_i(\mathbf{k})$  and  $f_i$  are momentum vectors, eigenvalues and Fermi factors in the bottom (B) and top (T) layers. The coupling matrix term  $O_{ij}(\mathbf{k}_B, \mathbf{k}_T)$  [13] represents the probability that a carrier can tunnel through a barrier from one momentum state into another:

$$O_{ij}(\mathbf{K}_B, \mathbf{K}_T) = \langle \psi_{iB}(\mathbf{K}_B) | V | \psi_{jT}(\mathbf{K}_T) \rangle. \quad (2)$$

where  $V$  is the scattering barrier potential of hBN and  $\psi_j(\mathbf{k})$  are BP monolayer states. In this work we have simulated a realistic barrier  $V$  from the local potentials computed in our LS-DFT simulations [7].

Two operating modes are shown in Figs. 2.c,d. In the first mode (Fig. 2.c), the TFET is in reverse bias, with valence electrons from the p-doped top layer tunnelling to unoccupied conduction states in the p-doped bottom layer. The subthreshold swing (SS), defined as the change in gate voltage required to increase the current tenfold, reflects the on/off switching capabilities. In MOSFETs, thermal carrier injection limits SS to a minimum 60 mV/dec, but in our TFET we observe lower SS, over six orders of current magnitude. This implies that a BP/hBN/BP TFET could switch between on and off states faster than any MOSFET, showing outstanding potential for high speed electronics. The second mode (Fig. 2.d) exhibits negative differential resistance (NDR) peaks [14], with known applications in oscillatory circuits and memory devices. The position of the NDR peak is highly tunable under modest gate voltages, due to the aligned energy levels of the BP films. The current generation is two-fold, between the bottom conduction electrons and the top unoccupied conduction states, and from the bottom valence electrons to the top holes. By perfectly aligning the bands through an increase in bias (point 2 in Fig. 2.d), a maximum number of tunnelling carriers is obtained, leading to a peak current. For even larger bias (point 3 in Fig. 2.d) the number of carriers is maintained, but the current drops due to the momentum-mismatch caused by the band misalignment, which decreases the coupling matrix terms  $|O_{ij}(\mathbf{k}_B, \mathbf{k}_T)|$ .

One has a choice between low- and high-power operation, since there are two means for large peak-to-valley ratios (PVR) to occur (right inset of Fig. 2.d): at low bias ( $V_{DS}$ ) for back-gate voltages ( $V_{BG}$ ) with the same sign as the top-gate voltage ( $V_{TG} = -1.00$  V), or at large bias for back-gate voltages of opposite sign as the top-gate voltage. The former case is energy-efficient due to low required bias, but the peak currents are also low. In the latter case, the peak currents and PVRs increase dramatically, but at the cost of larger gate bias voltages. Importantly, our obtained PVRs are of the same order of magnitude ( $\approx 2 \cdot 10^8$ ) as those predicted for TMDC/hBN/TMDC TFETs [15] ( $\approx 10^9$ ). These results imply that BP can be just as meaningful as TMDCs in TFET applications, as opposed to the case of MOSFETs where BP layers exhibit on/off current ratios [12] three orders of magnitude smaller than TMDC films [16].

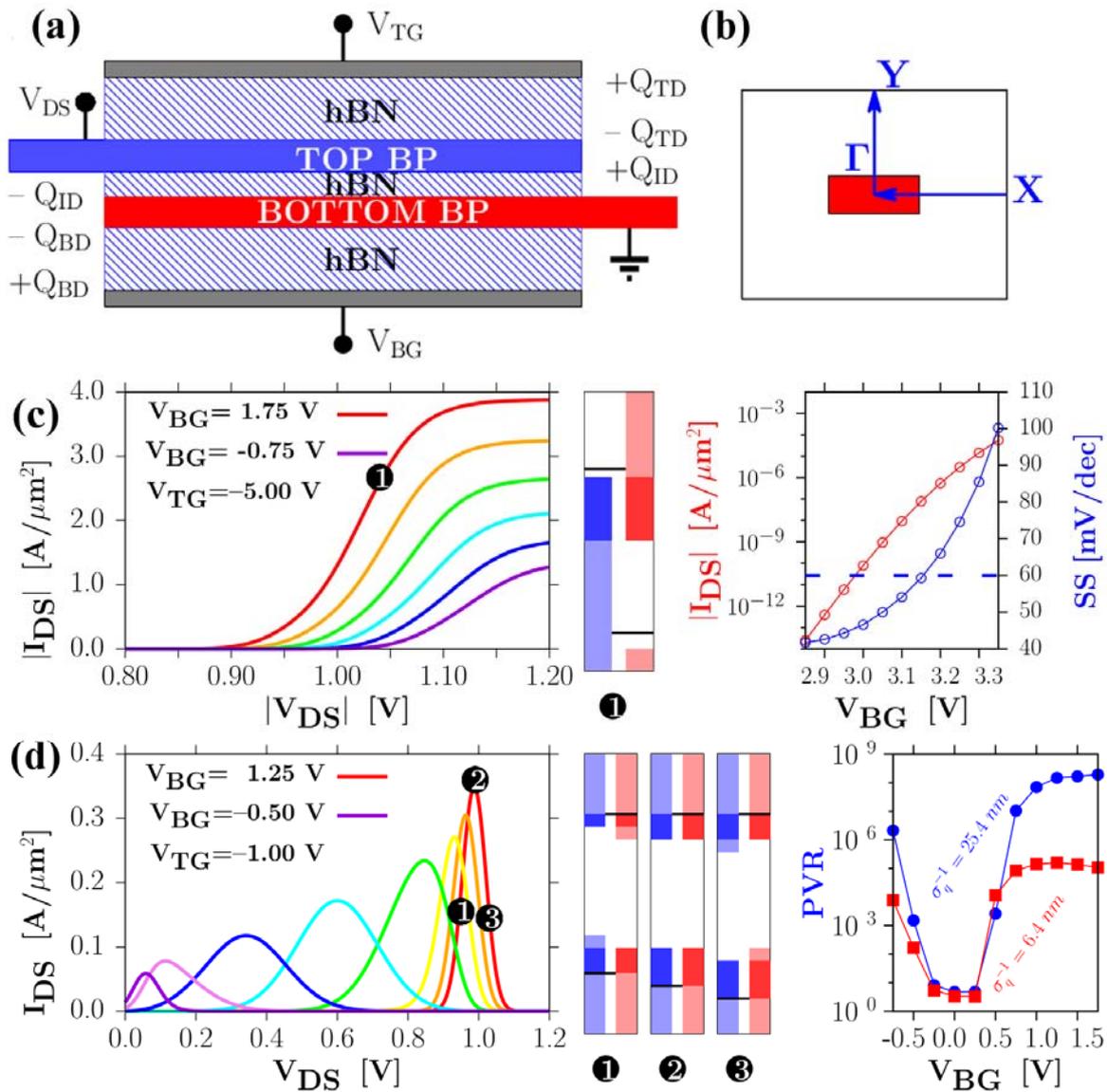


Figure 2: (a) Schematic of BP/hBN/BP transistor, with induced charges in the dielectrics. (b) The BP unit-cell Brillouin-zone. (c,d) Operation modes for the BP/hBN/BP TFET. The top-gate voltage ( $V_{TG}$ ) is fixed, band diagrams show energy levels of the top (blue) and bottom (red) BP layers – energy gaps are white, levels involved in tunnelling are darker, Fermi levels are black lines. (c) Left inset: current dependence for the reverse-bias regime. Right inset: current (red) and SS (blue) dependence on the back-gate voltage, at fixed  $V_{DS}=-0.6$  V; dotted line shows the MOSFET SS limit. (d) Left inset: NDR peak for the aligned-gap arrangement. Right inset: peak-to-valley ratios (PVR) for different back-gate voltages.

## TMDC interfaces

In this section we discuss the simulations of transition metal dichalcogenide (TMDC) heterostructures, performed alongside experiments at the University of Warwick and University of Washington, and published by Wilson et al. [17]. The unfolded spectral function once again illustrated band-structure alterations, now in stacks of different TMDC layers such as MoSe<sub>2</sub>/WSe<sub>2</sub> (Fig. 3). The simulated interface contained 873 atoms and had a rotation angle of 8.2°, similar to the experimental twists.

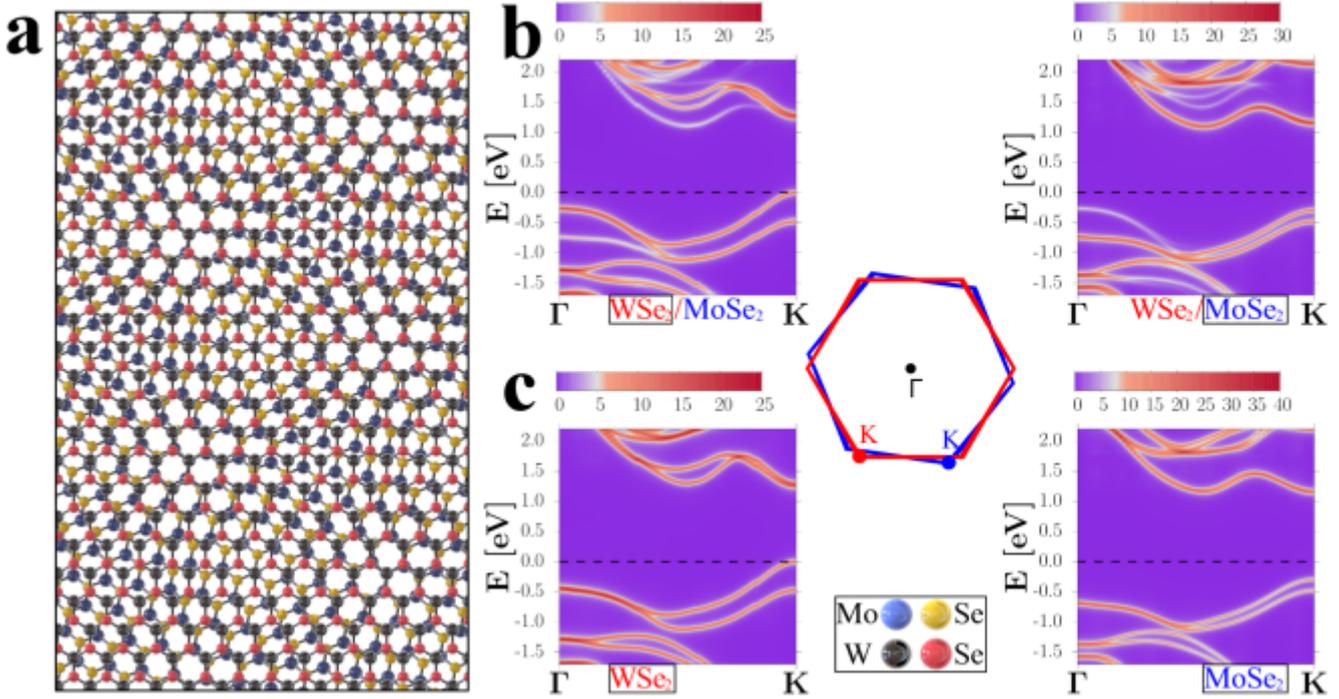


Figure 3: Misaligned MoSe<sub>2</sub>/WSe<sub>2</sub> interface (a). Unfolded spectral function projected on the stacked WSe<sub>2</sub> (b-left) and MoSe<sub>2</sub> (b-right) monolayers, as well as on the independent WSe<sub>2</sub> (c-left) and MoSe<sub>2</sub> (c-right) monolayers.

As already known, Fig. 3.c reveals the direct band gap at K for the independent monolayers. Comparing the electronic structure of the independent films (Figs. 3.c) with their stacked counterparts (Figs. 3.b), it is clear that stacking induces low spectral-weight bands protruding from one monolayer into the other. Furthermore, stacking interactions in MoSe<sub>2</sub>/WSe<sub>2</sub> (Figs. 3.b, c) raise the valence band maximum (VBM) at  $\Gamma$  of WSe<sub>2</sub> by 202 meV, and decrease the VBM of MoSe<sub>2</sub> by 67 meV. These trends are in line with the experimentally observed results [17]. Moreover, interlayer interactions are crucial for the correct modelling of band offsets. For instance, the valence band offset between WSe<sub>2</sub> and MoSe<sub>2</sub> is 0.29 eV, significantly lower than the 0.43 eV predicted by the independent-layer approximation [18], but in perfect agreement with the experimentally observed 0.30 eV [17].

## Commensurate and incommensurate domains

Experimentally, MoSe<sub>2</sub>/WSe<sub>2</sub> with a low twist angle ( $\approx 1^\circ$ ) exhibits an unusual behaviour: three highest valence bands at  $\Gamma$  (Fig. 4), instead of the expected two spin-degenerate bands for aligned MoSe<sub>2</sub>/WSe<sub>2</sub> [17] (Fig. 5, left inset). We believe the cause is the coexistence of commensurate and incommensurate phases occurring in the microflake. More precisely, we have previously shown [19] that in stacks of layers with similar lattice constant (such as MoSe<sub>2</sub> and WSe<sub>2</sub>) there is significant interlayer coherence only in for perfect alignment, whereas rotations induce decoupling to a large extent. The latter case would imply significantly less repelling (i.e. smaller energy difference) between the highest valence bands at  $\Gamma$ .

In order to prove our theory, we start with a simple but instructive approximation for the misaligned case. We have already shown in Fig. 3 that even with reduced interlayer coupling in incommensurate heterostructures, hybridisation always occurs near  $\Gamma$  between the bands of stacked monolayers. However, one could naively approximate the bandstructure of misaligned stacks as a simple superposition of the independent layers. We easily simulate this by starting from the commensurate maximally interacting case (“MC”,  $\Delta d = 0.0 \text{ \AA}$ ), and displacing the component layers until they are decoupled and the bandstructure stops changing (“D”,  $\Delta d \geq 2.0 \text{ \AA}$ ), as shown in Fig. 5. In the end, we

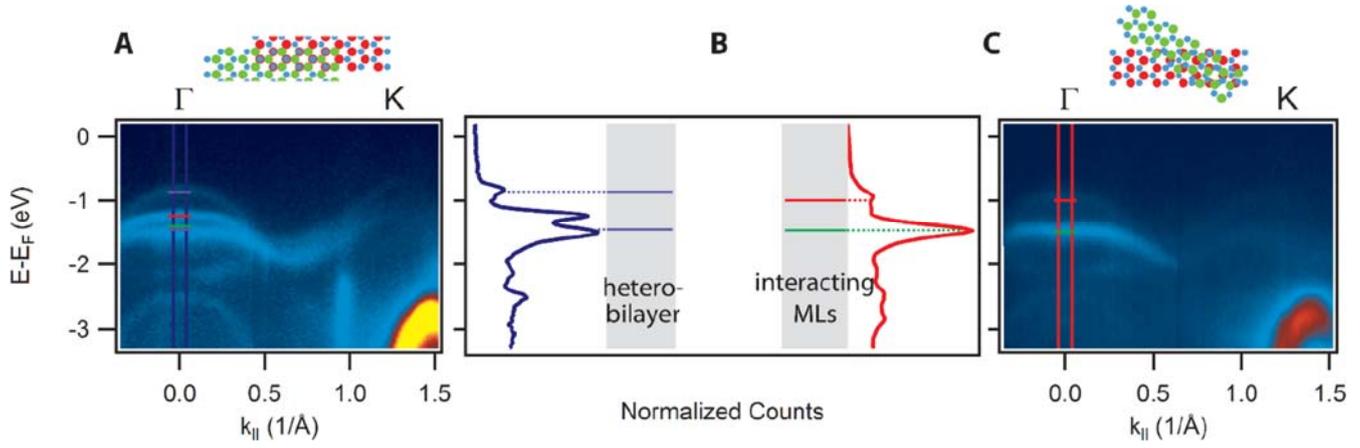


Figure 4: Courtesy of Wilson et al. [17]: ARPES slice along  $\Gamma$ -K for a nearly-aligned (A) and misaligned (C)  $\text{MoSe}_2/\text{WSe}_2$  interface. Energy distribution curve at  $\Gamma$  (B), and DFT predicted band positions at  $\Gamma$  of the purely commensurate heterobilayer (two blue bands) and interacting monolayers (two bands, red for  $\text{WSe}_2$  and green for  $\text{MoSe}_2$ ).

apply corrections (“D+”) to the independent-layer band edge positions as obtained from calculations on misaligned  $\text{MoSe}_2/\text{WSe}_2$  (Fig. 3), which specify that the  $E_{\text{HOMO}}^{\Gamma}$  of  $\text{WSe}_2$  is up-shifted by 202 meV in misaligned stacks, while  $E_{\text{HOMO}}^{\Gamma}$  of  $\text{MoSe}_2$  (i.e.  $E_{\text{HOMO}-1}^{\Gamma}$  of the heterostructure) is down-shifted by 67 meV.

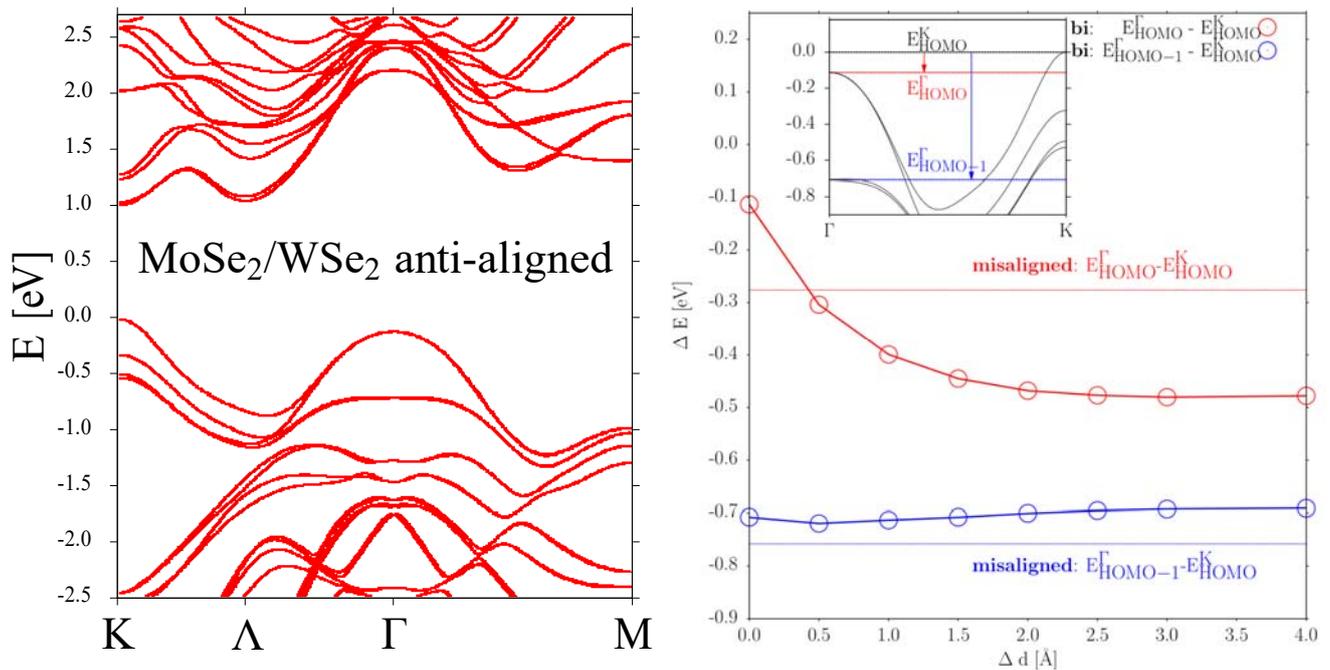


Figure 5: (left) Bandstructure of commensurate  $\text{MoSe}_2/\text{WSe}_2$ . (right) Changes in the highest VB energy at  $\Gamma$  for the perfectly anti-aligned  $\text{MoSe}_2/\text{WSe}_2$  bilayer. The inset shows levels for the commensurate interface, and the dashed lines represent the decoupled levels after being corrected for interactions in the misaligned interface.

It is clear that in both the “D” and “D+” cases, the energy differences between VBMs of the monolayers at  $\Gamma$  are significantly smaller than the ones at the “MC” state.  $E_{\text{HOMO}-1}^{\Gamma}$  remains at roughly the same position in all cases, while the VB at  $\Gamma$  ( $E_{\text{HOMO}}^{\Gamma}$ ) is by 340 meV lower in “D” or 138 meV lower in “D+” than it was at the

optimum interlayer distance. Thus, a superposition between the “MC” and “D” or “D+” would explain the 3 bands in the experimental ARPES measurements: the “D”/“D+”-state  $E_{\text{HOMO}}^{\Gamma}$ , the MC-state “ $E_{\text{HOMO}}^{\Gamma}$ ”, and lastly, a nearly-degenerate combination of  $E_{\text{HOMO}-1}^{\Gamma}$  from the “MC” and “D” or “D+” situations.

## Linear-response phonons in LS-DFT

We have developed a linear-scaling approach to linear-response phonons that is potentially suitable for large systems, such as our 2D heterostructures. The ultimate goal are Raman spectra calculations, which involve third-order energy derivatives with respect to atomic perturbations and electric fields. They can be proven to require only knowledge of the ground-state and first-order (perturbed) wavefunctions. Therefore, most of our effort went into determining the first-order wavefunction  $\psi_i^{1\lambda q}(\mathbf{r})$  in a linear-scaling manner where the subscript “ $1\lambda q$ ” implies a first-order atomic perturbation  $\lambda$  at wave-vector  $q$  of the ground-state wavefunction  $\psi_i(\mathbf{r})$ .

As ONETEP replaces delocalised eigenvectors through the use of localised optimisable atomic orbitals, we adhere to the same methodology by defining the first-order density matrix as:

$$\sum_i^{N/2} \langle \mathbf{r} | \overline{\psi}_i^{1\lambda q} \rangle \langle \overline{\psi}_i | \mathbf{r} \rangle = \sum_i^{N/2} e^{-i\mathbf{q}\cdot\mathbf{r}} \langle \mathbf{r} | \overline{\psi}_i^{1\lambda q} \rangle \langle \overline{\psi}_i | \mathbf{r} \rangle = \langle \theta_{\alpha} \rangle (\mathbf{P}^{1\lambda q \theta \phi})^{\alpha\beta} \langle \phi_{\beta} |, \quad (3)$$

where we have defined sets of localised atomic orbitals for the valence ( $\phi_{\beta}$ ) and response ( $\theta_{\alpha}$ ) manifolds, and a sparse response density kernel  $\mathbf{P}^{1\lambda q \theta \phi}$  that dictates the interaction between the aforementioned orbitals. The localisation of the orbitals and sparsity of the kernel ensure the linear-scaling behaviour of our approach [5]. For our implementation we have generally used the phase-factorised first-order eigenvectors  $\overline{\psi}_i^{1\lambda q}(\mathbf{r}) = e^{i\mathbf{q}\cdot\mathbf{r}} \psi_i^{1\lambda q}(\mathbf{r})$ , which have the periodicity of the simulation cell in spite of non-zero wave-vectors. Therefore, the optimal first-order wavefunction is determined by adapting the response kernel and response orbitals self-consistently.

Most existing algorithms use a conjugate gradient approach, but we are in a more difficult position due to the linear-scaling constraints. Our response-kernel optimisation problem can ultimately be expressed as a non-linear generalised Sylvester matrix equation:

$$\mathbf{A}^{\theta} \mathbf{P}^{1\lambda q \theta \phi} \mathbf{B}^{\phi} + \mathbf{C}^{\theta} \mathbf{P}^{1\lambda q \theta \phi} \mathbf{D}^{\phi} = \mathbf{E}_{\text{fixed}}^{\theta \phi} + \mathbf{E}_{\text{variable}}^{\theta \phi} \quad (4)$$

where the coefficient matrices  $\mathbf{B}^{\phi}$ ,  $\mathbf{D}^{\phi}$  rely only on ground-state quantities, while  $\mathbf{E}_{\text{fixed}}^{\theta \phi}$  depends on fixed first-order quantities independent of the first-order electronic density.  $\mathbf{E}_{\text{variable}}^{\theta \phi}$  is however a non-linear function of the first-order density, implying the need for a self-consistent optimisation scheme. We have thus implemented a quasi-Newton algorithm which minimises the Frobenius norm of Eq. 4. To speed up optimisation, we have also created an iterative preconditioning scheme, which allows us to achieve linear convergence, as seen in Fig. 6.

Once a suitable response kernel  $\mathbf{P}^{1\lambda q \theta \phi}$  was obtained for the current set of atomic orbitals, the response manifold  $\theta$  was also optimised using a preconditioned conjugate gradient scheme, essentially minimising the gradient of the second-order perturbation energy with respect to the  $\theta(\mathbf{r})$  functions:

$$\langle (g^{\theta})^{\eta} \rangle = \frac{\delta}{\delta \langle \theta_{\eta} |} \left[ \frac{d^2 E_{\text{OT}}}{d\lambda_{-q} d\lambda_q} \right], \quad (5)$$

Finally, in Fig. 6 we have verified our extensive implementation and theoretical framework by comparing our results to existing ONETEP finite-difference phonon calculations, as well as the linear-response phonons implementation in CASTEP [20]. Clearly we have almost perfect agreement with the CASTEP framework, which is implemented in a cubic-scaling manner, as opposed to our linear-scaling framework. There are some slight differences with respect to the finite-difference calculations, but this is expected because of the non-linear terms inherently included in the latter.

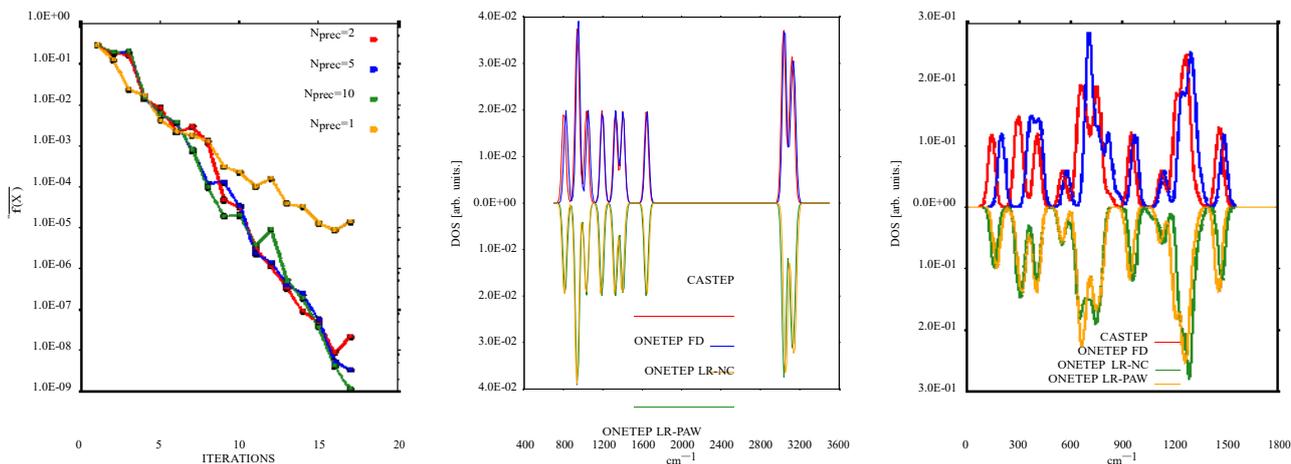


Figure 6: (left) Residual in quasi-Newton algorithm used for the response kernel optimisation, as a function of the number of preconditioning iterations. Vibrational density of states for an ethene dimer (middle) and a hBN monolayer (right). “NC” (“PAW”) indicates the use of norm-conserving (projector-augmented-waves) pseudo-potentials, while “FD” denotes finite-difference.

## Conclusions

We have shown that hBN encapsulation preserves the desirable electronic structure of monolayer BP, while hBN spacers counteract the band gap reduction in stacked BP, thus improving the efficiency of BP optoelectronics in the near-infrared. Furthermore, we have proposed and simulated a tunnelling field-effect transistor built from such spaced BP bilayers, with applications in ultra-fast switching and with large peak-to-valley ratios in negative differential resistance regimes.

We have also proven that LS-DFT applied to TMDC hetero-interfaces can explain bandstructure effects observed with experimental ARPES [17]. More specifically, we show that commensurate and incommensurate domains coexist in  $\text{MoSe}_2/\text{WSe}_2$  heterostructures with low-rotation angles.

Finally, we have derived the theoretical framework for linear-response phonon calculations in the LS-DFT framework of the ONETEP code. The constraints of localised orbitals and linear-scaling required developing innovative means of optimising the first-order wavefunction. Our results are in perfect agreement with existing methods, and they can potentially be used in large systems, such as two-dimensional heterostructures.

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# Computational Physics Group News

## • The Computational Physics Annual PhD Thesis Prize

Each year, the IoP Computational Physics Group awards a Thesis Prize to the author of the PhD thesis that, in the opinion of the Committee, contributes most strongly to the advancement of computational physics.

The winner of this year's Thesis Prize is Gabriel Constantinescu for his thesis entitled "Large-scale density functional theory study of van-der-Waals heterostructures", which was undertaken at the Cavendish Laboratory, University of Cambridge, UK.

The deadline for applications of the 2019 prize is 30th April and details are available at the following link:  
[http://www.iop.org/activity/groups/subject/comp/prize/page\\_40691.html](http://www.iop.org/activity/groups/subject/comp/prize/page_40691.html)

Applications are encouraged across the entire spectrum of computational physics. Entry is open to all students from an institution in the UK or Ireland, whose PhD examination has taken place since 1st January 2018 and up to the submission deadline, and who did not apply for the CPG Thesis Prize in the previous year. Prize winners will be invited to write a feature article in the Computational Physics Group newsletter.

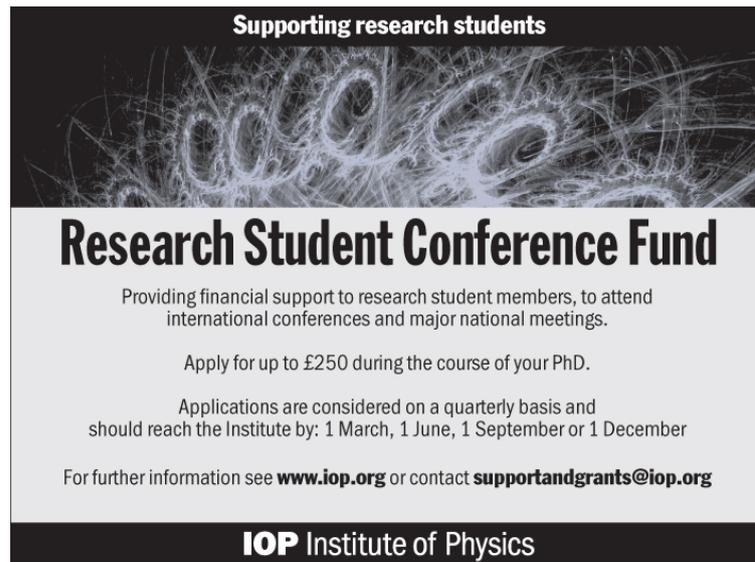
Candidates are asked to note that if a similar thesis prize is offered by another IOP group (such as the Theory of Condensed Matter group), the Committee intends to liaise with that group so that both prizes will not be awarded to the same applicant.

The submission format is as follows:

- A four page (A4) abstract describing the background and main achievements of the work
- A one page (A4) citation from the PhD supervisor, including confirmation of the date of PhD examination, that the student passed and whether the thesis has also submitted to another IoP group for a PhD thesis prize.
- A one page (A4) confidential report from the external thesis examiner

Entries (PDF documents preferred) should be submitted by email, with "IOP CPG Thesis Prize" as the subject header, to Dr Arash Mostofi ([a.mostofi@imperial.ac.uk](mailto:a.mostofi@imperial.ac.uk)). Any queries should also be directed to Dr Arash Mostofi. A few more details, including a list of past winners, can be found on the group webpage [http://www.iop.org/activity/groups/subject/comp/prize/page\\_40691.html](http://www.iop.org/activity/groups/subject/comp/prize/page_40691.html).

- IoP Computational Physics Group - Research Student Conference Fund



**Supporting research students**

**Research Student Conference Fund**

Providing financial support to research student members, to attend international conferences and major national meetings.

Apply for up to £250 during the course of your PhD.

Applications are considered on a quarterly basis and should reach the Institute by: 1 March, 1 June, 1 September or 1 December

For further information see [www.iop.org](http://www.iop.org) or contact [supportandgrants@iop.org](mailto:supportandgrants@iop.org)

**IOP** Institute of Physics

The Institute of Physics Computational Physics Group is pleased to invite requests for partial financial support towards the cost of attending scientific meetings relevant to the Group's scope of activity. The aim of the scheme is to help stimulate the career development of young scientists working in computational physics to become future leaders in the field.

Further details on this award can be found at:

[www.iop.org/activity/groups/subject/comp/prize/page\\_40691.html](http://www.iop.org/activity/groups/subject/comp/prize/page_40691.html)

## Conference and Workshop reports

- Fortran Joint Half Day Meeting, 28 September 2017

28 September 2017 at the BCS London Office in Southampton St.

Following the BCS Fortran Group's AGM in the morning of 28 September 2017 at the BCS London Office in Southampton St., a joint half-day meeting with the IoP Computational Physics Group was held. It was attended by 25 people, of which six declared themselves as IoP members. It was disappointing that only four were women. We began with an excellent buffet lunch, which gave us all an opportunity to get to know each other.

The first talk was on Coarrays in GNU Fortran by Salvatore Filippone of Cranfield University. In coarray Fortran, the program is replicated to a fixed number of images, usually processors, each of which has its own set of data objects. Some of these objects are coarrays, which means that they can be addressed from another image using 'cosubscripts' in square brackets. For example,

$$a(:)[k] = a(:)$$

copies the array  $a$  from the executing image to image  $k$ . The coarray language provides a clear syntax for parallel programming and is much easier to write and maintain than MPI. Since 2011, GNU Fortran has supported the syntax, but with execution limited to one image. From 2016, OpenCoarrays have supported most of the coarray features of Fortran 2008 on multiple images and are now supporting many of the extensions of Fortran 2018, including the ability to continue execution in the presence of a small number of failed images, quite likely during a long run on a huge number of images.



Wadud Miah of the Numerical Algorithms Group emphasized the importance of the Verification of Fortran Codes. As Fortran is the dominant language of HPC, compiler vendors have focused on producing performant code with little emphasis on correctness and language standards adherence. The presenter discussed the NAG compiler and its ability to catch common errors in Fortran codes which other compilers are unable to detect. A development workflow was presented which utilises static and runtime error checks in tandem with higher performant compilers to produce performance portable code. A recommendation was also made to encourage

code developers to openly publish the results of their unit tests and tool verification results to quantify the quality of their code.

Ian Chivers of Rhymney Consulting and Jane Sleightholme of Fortranplus reviewed how well current compilers comply with current standards. They introduced their document Compiler support for the Fortran 2003, 2008, TS29113 and 2018 standards which appears regularly in the ACM journal Fortran Forum.

John Reid, Convenor ISO Committee WG5, 1999-2017, provided a quick overview of the new features of the Fortran 2018 standard, which is expected to be published later this year. Because one of the suggested features for the next revision of Fortran in the new convenor's survey is Block-oriented or structured exceptions, John also described the exception handling feature that was included in 1994 drafts of Fortran 95, but was removed in November 1994 because it was seen as not ready and likely to delay Fortran 95.

Anton Shterenlikht of The University of Bristol spoke on Choosing the technical content for Fortran 2020 because a user survey was open. He provoked a lively debate on what changes are desirable. All the suggested changes were fed into the survey. Note that the committee (J3/WG5) does indeed listen to users. Another continuing feedback loop is via `comp.lang.fort`, which is read by the WG convenor and the J3 chair.

For more details on all these talks, see the abstracts and slides that are visible here:  
<http://www.fortran.bcs.org/2017/agenda17.php#present>.

Report kindly provided by Dr. John Reid

- **MCNEG 2018, University of Surrey and National Physical Laboratory, 30th January 2018**

30th January 2018 at the University of Surrey and National Physical Laboratory

The two day meeting of the UK Monte Carlo radiation transports codes took place at the University of Surrey on 30-31 January 2018. It was followed by a one day EGSnrc course led by Ernesto Mainegra-Hing of NRC Canada.

Ana Denis-Bacelar (National Physical Laboratory, NPL, UK) described Open Dose, a collaborative effort to produce reference dosimetric data from Monte Carlo simulations. 14 international teams are collaborating using a variety of MC codes, and is open to new collaborators. A web interface will be built to distribute these data freely. The FDA approved software phantoms Olinda had been freely available but was now part of a commercial package.

Frank Verhaegen (Maastricht) described small animal radiotherapy. A comprehensive review of treatment planning, dose painting and Monte Carlo verification was made. The rationale for this work was to improve research into radiotherapy treatments; radiotherapy is an unusual field in that novel treatments (eg IMRT) are introduced without first being tested on animals. This project aims to go beyond simple rectangular field irradiations. A customised small animal irradiator was described that uses Intensity Modulated techniques. Low energy beams (250 kV) were preferable to Megavoltage in animals as build-up effects could cause problems. Rob Shearman (NPL) discussed Measurements in radiation using  $\text{I}^{\text{137}}\text{-I}^{\text{137}}$  coincidences for absolute standardisations. The National Nuclear Array (NANA) is a twelve detector array of detectors that is used for absolute measurements that can be compared with a primary standard.

Angular corrections were carried out. The NPTool was used for analysis; this uses Geant routines and is a publicly available toolkit. The angular correction means NANA is comparable to 4 pi measurement systems.

Michael Hubbard (NPL) looked at pulse shape discrimination in plastic scintillators. Geant4 was used to model optical and radiation transport. He set up a working Geant4 model of a scintillator which tracks optical photons. Then he validated the model against common scintillator detector and expanded the model onto plastic scintillator. He then modeled a scintillator with pulse shape discrimination abilities in order to investigate experimentally observed degradation.

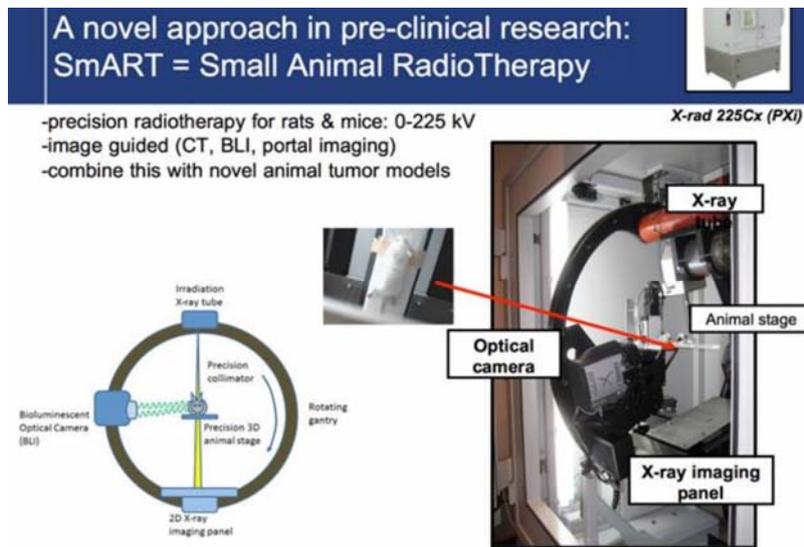


Figure 1: Small Animal Irradiator

Mohamad Qutub (Swansea) looked at modelling linac rooms using Fluka. He referred extensively to Al-Affan's estimates of the effect of the presence of a patient on the energy spectrum of leakage radiation at the maze entrance. He used a Fluka with an algorithm using a Poisson distribution to correct pulse pile-up in the sodium iodide and plastic scintillators used to measure the photon spectrum at the maze entrance.

Henry Lawrence described a visit by 16 UK physicists to the site of the Chernobyl nuclear reactor. A GPS enabled contamination monitor built by David Muoat (Newcastle) was tested to create a map of contamination. The tour gave a most interesting look at the effect of a catastrophic nuclear accident, and also gave a first hand glimpse into life in the Soviet Union. Ernesto Mainegra-Hing spoke about modelling electrons in magnetic fields. The advent of the MRI linac has made this an important topic. The EGSnrc algorithm used approximates the tracks with polygons of ever increasing resolution to approximate the curved motion of the tracks. Fano's theorem does not hold in the presence of static and constant external EM fields. This has the unfortunate consequence of invalidating the Fano cavity test. Errors of about 20% were reported, and this effect was studied in detail.

Peter Sitch (Christie) carried out checks on clinical proton radiotherapy plans calculated by the Eclipse treatment by comparing them with Gate / Geant4 computations. The beam components (depth dose, beam optics, range shifter) were modelled. Discrepancies greater than 20% Outstanding issues include validation of ionisation potential and large scale validation of clinical plans. Legal aspects of QC using a bespoke tool were discussed.

Christopher Green (NPL) discussed electron ionisation chamber perturbation factors. These were calculated using DOSXYZ for the Roos and NACP 002 chambers that are commonly used as field chambers in the UK. The calibration chain starts with dose to graphite calorimeter, then dose to chamber in graphite, then dose to chamber in water. An accurate model of the NPL beam was built using BEAM, the reference depth established. Then chamber walls and cavity were replaced with water in the model to generate perturbation factors. Richard Hugtenberg discussed scatter induced range uncertainty problems resulting from the effect small structures in bone (and in Sawbone, a bone phantom material). The effect broadens a proton beam Bragg peak. This problem may be more significant in lung tissue. The variations in position of the Bragg peak were computed using FLUKA and were experimentally verified with radiochromic film. High spacial MRI sequences have been developed to characterise the substructures. John Cotterill (Birmingham) described a Geant4 simulation of a proton imaging system for measuring average energy loss. The PraVDA consortium has developed a range telescope, but this was too big to be used in a clinical setting. A Geant4 model was built of the range telescope and a balsa wood phantom simulated in the 36MeV Birmingham Cyclotron beam. The calibration

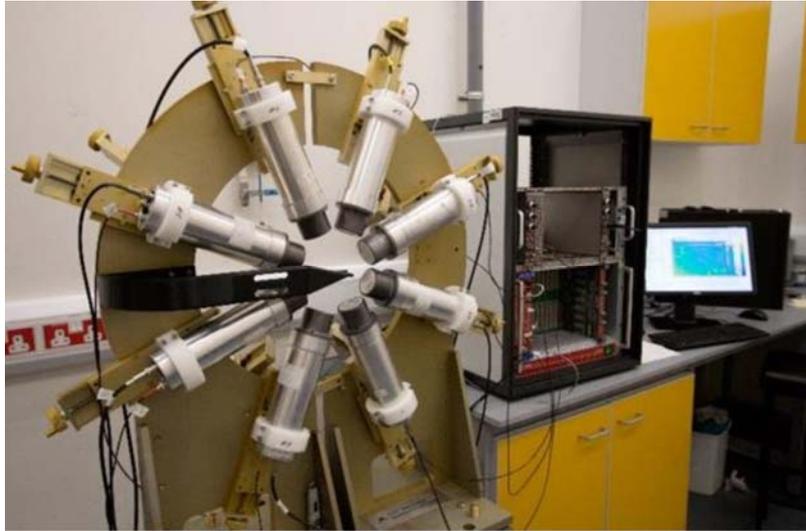


Figure 2: National Nuclear Array (NANA)



Figure 3: The Chernobyl explosion

was performed using perspex sheets, and an average energy was obtained from the water equivalent path length.

Dmitri Reynard (Swansea) spoke about a Monte Carlo intercomparison of PVDR (peak to valley dose ratio) and OF (output factor) for Microbeam Radiotherapy. This research modality uses 50 micron synchrotron beams with a very high dose rate (15000 Gy/s) to create fields with large dose variations.

Initial reports indicated large OF discrepancies ( 10%) between codes. This work compared Geant4, EgsNRC and Penelope, and OF differences were reduced to 4% between EgsNRC and Geant4. Discrepancies seem to be due to the way Compton scattering is handled by different codes., and als by differences in electron transport in low density materials. A PTW Microdiamond detector was used to verify the results; the validity of the reciprocity theorem for the Microdiamond was investigated.

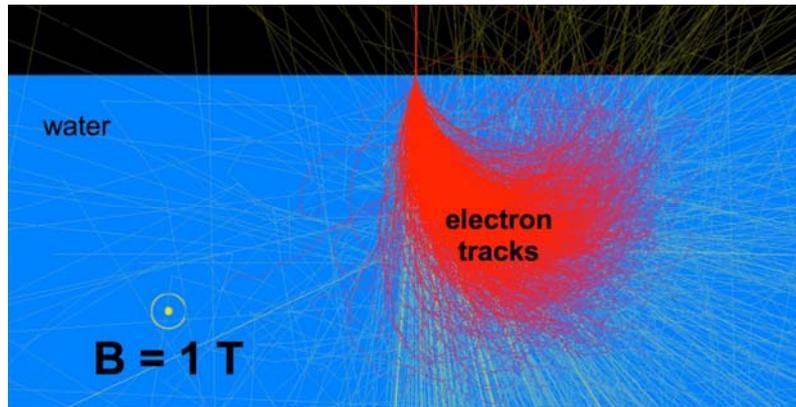
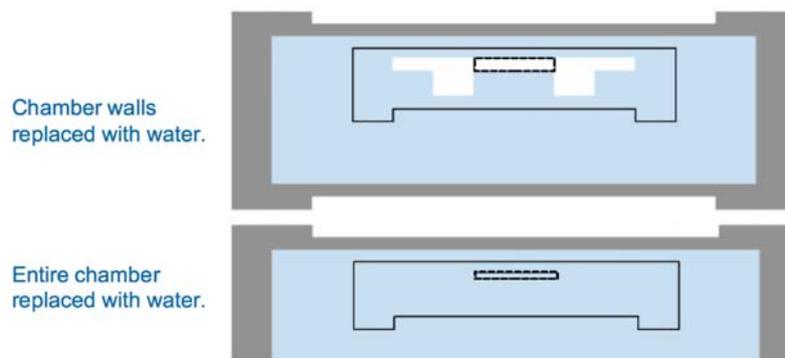


Figure 4: Electron tracks in a 1 tesla field

## Replacing the Chamber Walls and Cavity



Ilias Billas (NPL) discussed “Working towards dosimetry of MRI guided linacs”. MRI guided linacs will improve imaging during treatment without adding to normal tissue patient dose. A correction factor is described that changes absolute dose by about 0.4% in a 1.5T B-field. Alanine dosimetry and ionisation chambers were used for verification. Fano theorem tests were carried out to ensure results were density independent.

Carla Winterhalter (Paul Scherrer Institute, Switzerland) described scanned proton pencil beam simulations they carried out in comparison with work done at the Christie Hospital, UK using Geant4 and Topaz. An interesting discrepancy arose due to different ionisation potentials for water that arose if the user used the elemental composition of water or the recommended water value. Physical and software wedge shaped phantoms were described. Final agreement between both centres and measurements was good (within 2.5

Finally, for the evening’s entertainment, Jammie Sammy entertained delegates with her extremely witty songs about Ninja Crabs and the like.

Many thanks to Seb Galer for organising this excellent meeting and course ,and to the IoP for its generous contribution.

Report kindly provided by Dr. John Reid

- Software Carpentry conference, Dublin 2018, 30th May - 1st June  
30th May - 1st June in Dublin, Republic of Ireland

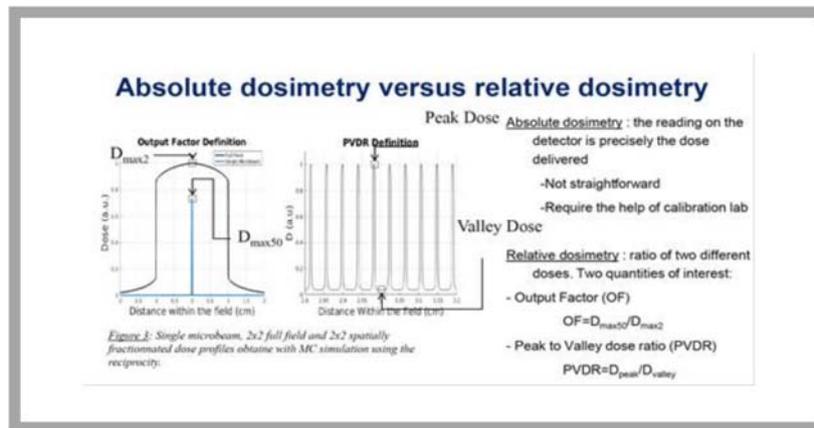
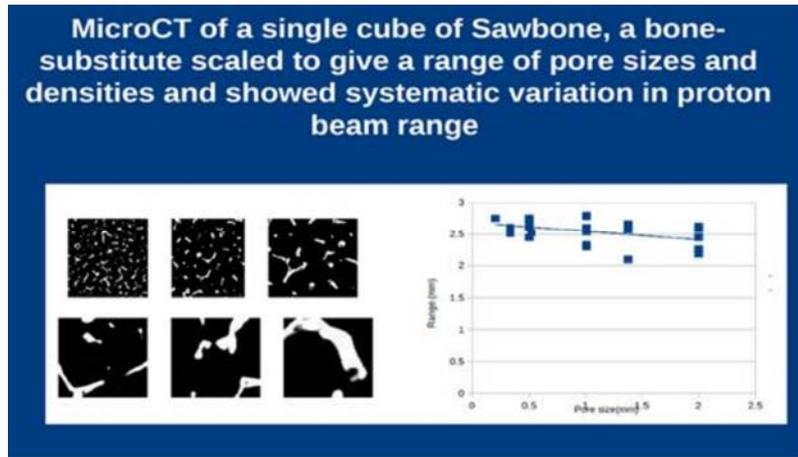


Figure 5: Microbeam dosimetry

Highlights. At the end of May I attended the Software Carpentry conference in Dublin. Software Carpentry is a volunteer organisation that teaches basic programming skills to researchers. Last year I trained as a Software Carpentry instructor and, as the majority of this process was online, I was keen to meet my colleagues in real life. Many of the conference attendees work within universities as researchers or research software engineers; there were also people from organisations such as the Software Sustainability Institute and Edinburgh Parallel Computing Centre. For me, the highlight of the programme was hearing about the development of the Clustal multiple sequence alignment programme that was first developed in the late 1980s. The developer Des Higgins (who wrote one of Nature's top ten most cited papers of all time) spoke about Clustal's success being due to good documentation and free distribution. He reminisced about packing up floppy disks and posting them across the world – luckily, sharing code is much easier now! It was nice to hear evidence that the good practice Software Carpentry promotes, such as producing solid documentation, does make an impact on the quality of research. The conference programme included several discussion sessions. One of these was focused on the development of intermediate level courses, which would include topics such as automated testing and modular code development. I am currently integrating these practices into my own code development and, as I have found the best way to learn something is to teach it, I was keen to get involved. After being introduced to resources developed for the code refinery project (<http://coderefinery.org>), I am planning to teach an adapted version of this course in the future. This conference was different to the majority of conferences I have been to. It was wide in scope, with talk topics ranging from computer science to education to diversity and inclusion. It was great to meet a large group of nerdy people who like to share things, as one attendee put it. I look forward to the next one.

Report kindly provided by Lucy Whalley, Imperial College London, June 2018.

### **46<sup>th</sup> IOP Plasma Physics Conference**

The IOP Computational Physics Group is sponsoring this event on 23-26th April 2019 in Loughborough, UK.

<http://plasma2019.iopconfs.org/home>

The annual IOP Plasma Physics Conference covers all aspects of plasma physics, including Magnetic and Inertial confinement fusion, Astrophysical and Space Plasmas, Low Density and Technological/Industrial Plasmas, Low Temperature Plasmas, High Energy Density and Laser Plasmas, Dusty and Complex plasmas, Plasma Surface interactions, Plasma Applications including Medical applications and Plasma Diagnostics. This year, the conference will be collocated with the 3rd UK Pulsed Power Symposium.

Registration deadline is 12th April 2019

### **The POP EU Project – A free of charge service within the EU to analyse performance of parallel software, identify issues and assess performance improvements**

NAG are delighted to be part of the POP (Performance Optimisation and Productivity) EU project that is helping to improve the performance of software. In brief POP offers to analyse software and recommend improvements with a focus on HPC and parallelisation. This service is free of charge to people within the EU.

We have the tools and expertise to analyse all aspects of code performance from individual CPUs up to inter-processor communications, for example successfully identifying memory bottlenecks and load imbalances for existing clients, allowing a better understanding of execution efficiency and targets for code refactoring.

We're currently identifying new users for whom software performance improvements could lead to benefits for the organisation or user community. To express an interest please contact [pop@nag.co.uk](mailto:pop@nag.co.uk) or see the POP website for more information <https://pop-coe.eu/>.

*Report kindly provided by Sally Bridgewater, Numerical Algorithms Group, Oxford, UK, November 2018.*

## Upcoming Events of Interest

Upcoming events of interest to our readers can now be found via the following web links.

- IOP's index page for scientific meetings, including conferences, group events and international workshops:

[www.iop.org/events/scientific/index.html](http://www.iop.org/events/scientific/index.html)

- IOP Conferences page for conference information, calendar and noticeboard:

[www.iop.org/events/scientific/conferences/index.html](http://www.iop.org/events/scientific/conferences/index.html)

- All events being run or supported by IOP Groups including calendar and links to event web pages:  
[www.iop.org/events/scientific/group/index.html](http://www.iop.org/events/scientific/group/index.html)
- Thomas Young Centre: The London Centre for Theory and Simulation of Materials organises many different kinds of scientific events on the theory and simulation of materials, including Highlight Seminars, Soirees and Workshops. For further details of upcoming events please visit:  
[www.thomasyoungcentre.org/events/](http://www.thomasyoungcentre.org/events/)
- CECAM is a European organization devoted to the promotion of fundamental research on advanced computational methods for atomistic and molecular simulation and their application to important problems in science and technology. CECAM organises a series of scientific workshops, tutorials and meetings. For further details please visit:  
[www.cecarn.org](http://www.cecarn.org)

## 44th NI Physics Teacher's Conference 2019

This celebrated and highly valued conference is organized by IOP NI Physics Teacher Network Coordinators in Northern Ireland. This event is one that features presentations and workshops and is open to all teachers of physics – specialists, non-specialists, newly qualified and trainee teachers. This year it is being held in Armagh Observatory in Northern Ireland. The IOP NI Physics Teacher Network offers free CPD, support and advice to teachers of physics. The Network is made up of more than 40 Physics Network Coordinators, located throughout the UK and Ireland. These coordinators are all very experienced teachers, or former teachers, who act as consultants to the IOP and work to support local teachers. The coordinators organise free CPD workshops, conferences and events for teachers in their area. They act as a source of information about local initiatives and activities, and generally provide help and advice in response to requests. They also help to forge better links between school sectors, and between schools and HE.



Further details available at: <https://www.eventbrite.co.uk/e/44th-ni-physics-teachers-conference-2019-armagh-tickets-61729316046>

Date: Thursday, 20 June 2019