

## Gap engineering in atomically thin materials

James P. Hague

Department of Physical Sciences, The Open University, Walton Hall, Milton Keynes, MK7 6AA, UK  
J.P.Hague@open.ac.uk

A perturbative theory is presented for the strong enhancement of graphene-on-substrate bandgaps by attractive interactions mediated through phonons in a polarizable superstrate. By constructing a set of self-consistent equations, it is demonstrated that gaps of up to 1eV can be formed for experimentally achievable values of electron-phonon coupling and phonon frequency [1]. As shown in figure 1, gap enhancements computed using perturbation theory range from 1 to 4, indicating possible benefits to graphene electronics through greater bandgap control for digital applications, through the relatively simple application of polarizable materials.

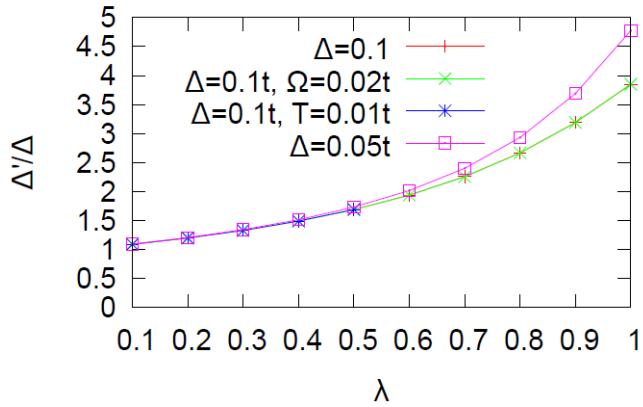
Additionally, polaron spectral functions are computed for heavily doped graphene-on-substrate systems using the diagrammatic quantum Monte Carlo technique to investigate the effects of interaction on spectral functions when the symmetry between graphene sub-lattices is broken by a substrate [2]. Several polaronic features are visible, including band-flattening and changes in particle lifetimes. The difference between energies on each sub-lattice increases with coupling, indicating an augmented transport gap at the K point, while the spectral gap decreases slightly (as shown in figure 2). In the absence of a gap, additional flattening is found around the K point.

I also discuss the effects of substrates on atomically-thin graphene-like materials such as boron nitride (BN) and silicene. To cope with more complicated momentum-dependent interactions that may be formed between electrons and phonons within monolayers, I reintroduce momentum dependence to the perturbation theory. Gap enhancements are reassessed, and useful forms of the interaction for gap tuning are identified.

## References

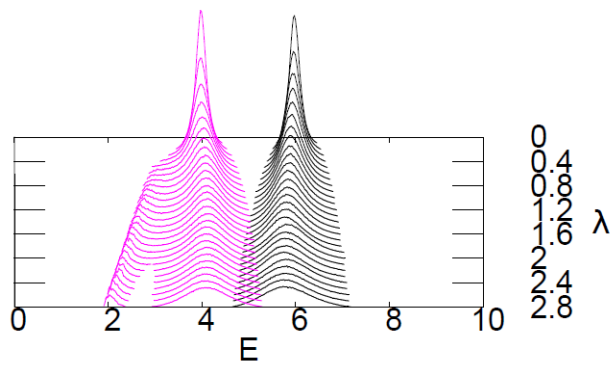
- [1] J.P.Hague. Tunable graphene band gaps from superstrate-mediated interactions. Phys. Rev. B, **84** (2011) 155438.  
 [2] J.P.Hague. Polaron effects in heavily doped graphene on substrates. arXiv:1107.2507 (2011)

## Figures



**Figure 1: Substrate gap enhancement vs superstrate mediated electron phonon coupling  $\lambda$ .  $\Delta$  is the non interacting gap,  $T$  the temperature,  $t$  the hopping and  $\Omega$  the phonon frequency.**

$A(E)$



**Figure 2: Spectral function,  $A(E)$ , for heavily doped graphene at the K point.**