Improving on two-dimensional materials?

First principle investigation of functionalization of transition metal dichalcogenides

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In Short

- Exploring functionalization of transition metal dichalcogenides
- Effects on electronic and optical properties
- Effects of defects in the transition metal dichalcogenides
- Inclusion of electronic correlations via GW approach
- Exitonic effects via the BSE approach

Given the success of dye-sensitized solar cells employing TiO_2 supports, it is reasonable to assume that the optical properties for other substances like transition metal dichalcogenides (TMDCs) might be further enhanceable via targeted molecular functionalization. Our project is focussed on the electronic structure of TMDCs with defects and their exciton binding energies. We will determine the change in the electronic properties which is caused by functionalization using advanced first principle methods. Functional molecules will be absorbed to TMDCs at the most common type of defect, the S-vacancy[1] [2] . This functionalization will promote the development of two-dimensional devices for molecular recognition like gas-sensing applications and for optoelectronic applications. We intend to investigate MoS_2, $MoSe_2$, WS_2, WSe_2 to see the influence of the used chalcogenide and the transition metal.

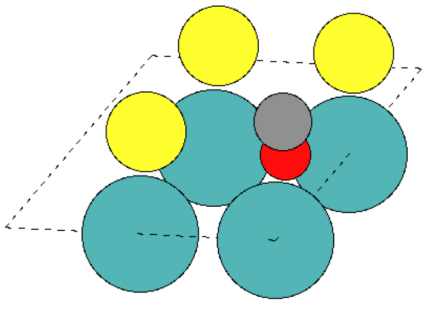

Figure 1: *CO adsorbed on a MoS_2 2x2 supercell with one S vacancy*

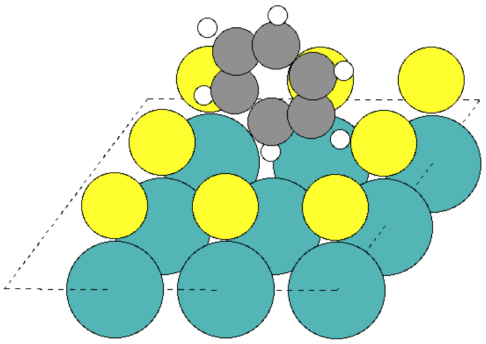

Figure 2: *Benzene adsorbed on a MoS_2 3x3 supercell with one S vacancy*

While the bare TMDC's materials have been widely discussed in the literature, even including S vacancies little is known about the effect of adsorption of molecules on the electronic structure. Herein we will investigate the adsorption of different molecules, which can be used as anchoring groups for functionalization on defective and defect-free TMDCs. For this part we will employ vdW-DFT to accurately account for the weak interactions between the substrate and the adsorbed molecules. We will study the energetic and electronic properties of systems using recently developed methods to incorporate screening effects within vdW-bound systems [3] to study the effects of adsorption on the electronic structure of the TMDCs within the G_0W_0 approximation. Excitonic effects will be considered within the use of the Bethe-Salpeter-Equation (BSE).

WWW

http://www.bcp.fu-berlin.de/chemie/

More Information

[1] S. McDonnell, R. Addou, C. Buie, R.M. Wallace, C.L. Hinkle, *ACS Nano* **8**, 2880 (2014). doi:10.1021/nn500044q

[2] H. Qiu, T. Xu, Z. Wang, et al. *Nat. Commun.* **4**, 2642 (2014). doi:doi:10.1038/ncomms3642

[3] K. T. Winther and K. S. Thygesen, *2D Mater.* **4**, 2 (2017). doi:10.1088/2053-1583/aa6531

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