Modeling vertical and lateral electron transport across heterostructures of 1D and 2D materials.

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I will present recent developments made in the understanding of charge transport across heterostructures between nanostructured materials, including one-dimensional and two-dimensional graphene- and transition metal dichalcogenide- based systems.

The first part of the presentation will focus on electron transport taking place along on-dimensional heterostructures [1]. I will show how controlled chemical doping on one side of the junction can lead to physical properties that are well suited for photovoltaics and photocatalysis device development. In addition, it will be demonstrated that the appropriate choice of monomers used in the bottom-up assembly of these materials can yield tunable properties.

The second part of the talk will be devoted to a description of the role of collective motion in the ultrafast charge transfer in van der Waals (vdW) heterostructures. [2] Using time-dependent density functional theory molecular dynamics, it was found that the collective motion of excitons at the interface of the vdW heterostructures leads to plasma oscillations associated with optical excitation. Application to the experimentally realized MoS_2/WS_2 heterostructure yields good agreement with experiment, indicating near complete charge transfer within a timescale of 100 fs.

Finally, I will briefly present recent theoretical developments in the understanding of electronic band gap renormalization induced by substrate polarization effects, taking adsorbate size into account.

[1] J. Cai *et al.*, Nat. Nanot. **9**, 896 (2014); A. Lherbier *et al.*, Carbon **95**, 833 (2015); L. Liang and V. Meunier, J. Phys. Chem. C **119**, 775 (2015).
[2] L. Liang and V. Meunier, Nanoscale **6**, 5394 (2014); S. Huang *et al.*, Nano letters **14**, 5500 (2015). H. Wang, *et al.* Nature Communications, 7, 11504 (2016).
[3] N. Kharche and V. Meunier, J Phys Chem Lett. 7(8):1526-33 (2016)