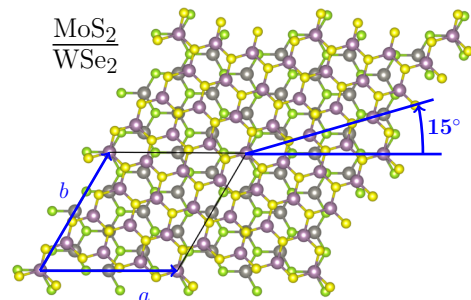


Modeling the properties of van der Waals heterostructures of 2D materials

František Karlický

Department of Physics, Faculty of Science, University of Ostrava, 30. dubna 22, 701 03, Ostrava, frantisek.karlicky@osu.cz

Research on graphene and other two-dimensional (2D) atomic crystals is currently very intensive and is likely to remain one of the leading topics in condensed matter physics and materials science for many years to come. Isolated atomic planes can be further reassembled into heterostructures, built up layer by layer in a precisely chosen order (often therefore referred to as “van der Waals” heterostructures) [1]. Recently prepared heterostructures have revealed a huge diversity in their properties and have also shown new phenomena and possibilities for technological devices for (nano)electronics and photovoltaics [2]. First-principles calculations also help to understand the possibilities of heterostructures. However, in 2D materials, due to the weak dielectric screening from the surroundings, the effects of electron-electron and electron-hole (exciton) interactions are specifically enhanced, so the popular density functional theory (DFT) method is usually insufficient for modeling more advanced properties. The state-of-the-art methods for reliably predicting fundamental band gaps and optical properties of materials are the many-body perturbation approximation GW and the Bethe-Salpeter equation (BSE), which have proven effective in various 2D and layered materials [3-5]. Although well-executed GW+BSE calculations can predict delicate phenomena such as the 2D exciton insulator [6] or stacking-dependent interlayer excitons [7], the approach remains very demanding in terms of computational time and memory, and its application to larger computational cells is almost impossible while maintaining accuracy. We have recently shown that time-dependent density functional theory (TD-DFT) based on a specific hybrid density functional can approximately take into account all important physical effects, including excitons [8-9], and therefore is a practical technique for van der Waals heterostructures containing incommensurate cells of different monolayers, allowing, for example, a detailed analysis of layer and interlayer excitonic wave functions [10].



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