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Theoretical studies of two dimensional systems

Since the discovery of graphene in 2004, many new 2 dimensional materials have been synthesised. These form ideal systems to model quantum mechanically and to modify computationally, for example by doping or the creation of various defects, with the view to alter the physical, electronic, magnetic, etc., properties. Within the framework of density functional theory, a number of 2D systems will be discussed for their often unique and novel properties. In addition, a new theoretical scheme will be presented that enables the computation of the elastic properties of these materials.

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