Heterostructures of two-dimensional transition metal dichalcogenides: Formation, ab initio modeling and possible applications

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Abstract: State-of-the-art technologies of fabrication of monolayers of transition metal dichalcogenides like MeX_2, where Me = Mo, W; X = S, Se, Te, and their based heterostructures are considered. Results of theoretical modeling are analyzed and possibilities of band gap engineering by means of strains, impurities, vacancies, various layer stacking and combination of different materials are presented. Vacancies

and impurities in the positions of metal atoms are shown to drastically change the band gap, even leading to an appearance of metallic properties, whereas a substitution of chalcogen atoms by isovalent atoms changes the properties not so dramatically. Possible applications of heterostuctures with tunable band gaps in transistors, light-emitting diodes, photoelectrochemical cells or photovoltaic devices are proposed and their advantages in comparison with commonly used analogues are discussed.

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