chem2Dmat
September 03-06, 2019 ● Dresden, Germany
European Conference on Chemistry of Two-Dimensional Materials

Dependence of bonding, structure, and performance of monolayers on the position in the periodic table

Peter Hess

University of Heidelberg, Institute of Physical Chemistry, INF 69120, Heidelberg, Germany
peter.hess@urz.uni-heidelberg.de

Covalent bonding and the resulting two-dimensional (2D) structure vary widely within the large family of 2D materials. They control chemical stability, critical strength, and toughness of the chemically bonded network. These properties, which determine stability and durability under mechanical forces occurring during applications are not yet well known. For any application chemical and mechanical properties are crucial including manufacturing, integration into devices, and performance during operation. For a meaningful comparison of mechanical behavior 2D units must be used, which can be measured directly and do not need knowledge of the monolayer thickness. Nevertheless, the layer thickness or monolayer volume is needed to transform 3D units into 2D properties and to estimate multilayer properties. It is shown that van der Waals diameter-based thickness values should be used instead of calculated or measured interlayer distances in the case of strong interlayer interaction (see Fig. 1).

To obtain a sufficiently complete picture over the whole 2D family chemical relationships existing along the columns of the periodic table can be employed to predict missing information, especially in the case of heavier compounds [1,2]. It is shown, how such estimates can be achieved on the basis of widely available linear properties, such as Young's moduli (see Fig. 2). As outcome linear and nonlinear mechanical properties are provided for single-atom elemental monolayers of group III, IV, V, and VI elements and their binary compounds, as well as mixed group III–V and group IV–VI monolayers. Within the second row of the periodic table boronitrene and graphene exhibit the strongest covalent bonding with exceptional properties, whereas within the columns of the periodic table stiffness and critical strength deteriorate extensively from the light elements to the heavier and larger atoms. Chemical reactivity is a serious problem for compounds with mixed hybridization, because partially covalent interaction ('dangling bonds') takes place at the surface that must be avoided by passivation. An overview on the type of bonding and resulting stability is provided.

[1] P. Hess, Nanotechnology, 28 (2017) 064002.

[2] P. Hess, Phys. Chem. Chem. Phys., 20 (2018) 7604–4611.

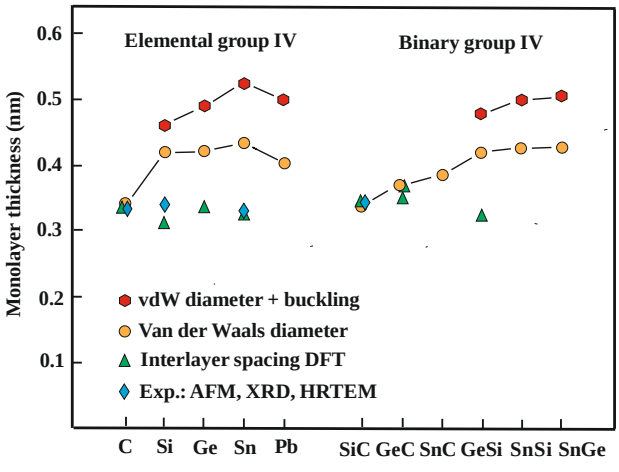

Figure 1: Layer thickness approximated by van der Waals diameters, calculated, and measured interlayer distances of group-IV compounds.

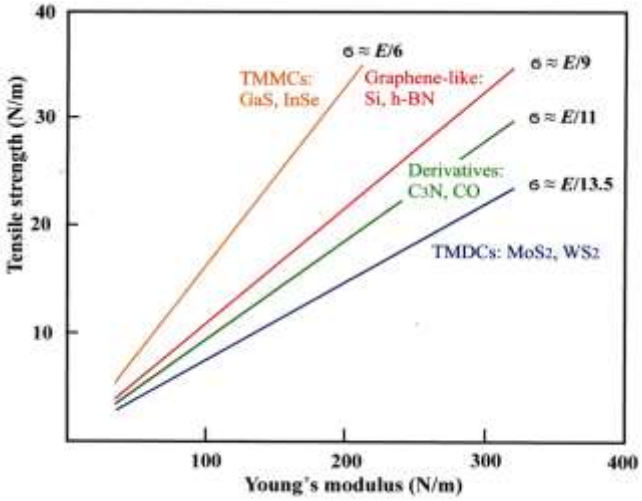

Figure 2: Correlation of Young's modulus E and tensile strength σ of transition-metal monochalcogenides, graphene-like mono-layers, graphene derivatives, and TMDCs.