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A Semi-Empirical Approach to Bandstructure, Chemistry and Transport: Extended Hückel Theory applied to Carbon Nantotubes and Silicon -[1] DIEGO KIENLE, Purdue University, JORGE CERDA, Instituto de Ciencia de Materiales de Madrid, KIRK BEVAN, Purdue University, GENGCHIAU LIANG, Purdue University, LUTFE SIDDIQUI, Purdue University, AVIK GHOSH, University of Virginia, M.P. ANANTRAM, NASA Ames Research Center — We apply semi-empirical Extended Hückel Theory (EHT) to calculate electronic structure and zero bias density-of states and transmission for two technologially important materials: carbon nantotubes and silicon. We demonstrate that the EHT-parameters optimized for bulk-silicon and 2D-graphene are transferable to describe qualitatively and quantitatively the electronic structure of structural deformed systems such as small diameter CNTs and relaxed silicon surfaces for different orientations. Finally, we show that the non-orthogonal EHT-approach can handle electronic structure and bonding chemistry simultaneously considering a carbon-monoxide-CNT heterostructure as example for a molecule sensor.To study transport through large nanoscale devices along with attached molecules a semi-empirical approach such as EHT might offer a good compromise between computational expensive DFT-methods and effective mass models which do not capture molecular features.

[1]DURINT

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