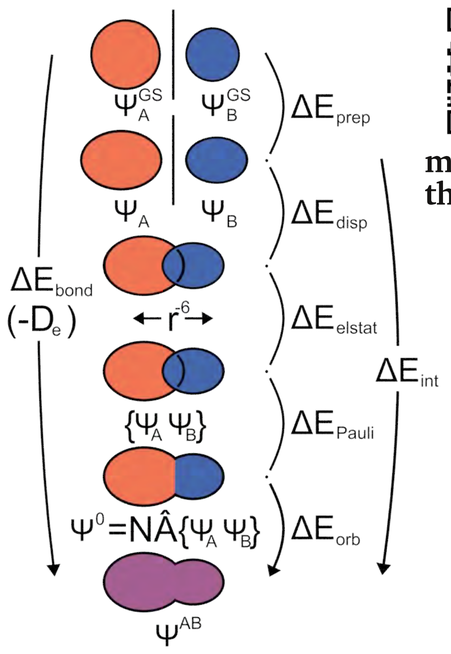
Theoretical Chemistry of Complex Matter

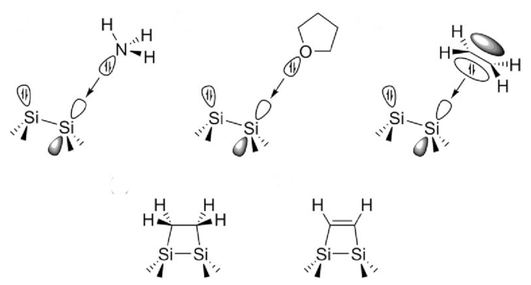
UNIVERSITÄT LEIPZIG

Tonner-Zech Group
Wilhelm-Ostwald-Institute

The Chemical Bond

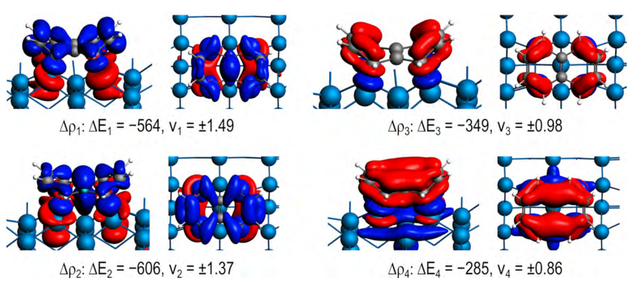


Understanding bonds between atoms or molecular fragments is at chemists heart. The energy decomposition analysis splits the bonding energy between two fragments in physical meaningful contributions. Thereby the nature of the chemical bonds can be investigated.

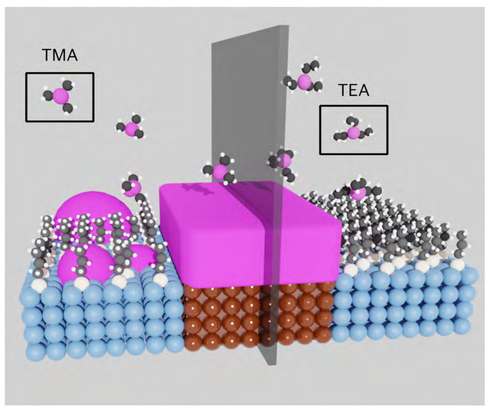


Covalent bonds? Dative bonds? Ionic or Van-der-Waals bonds? Also for the adsorbate surface interaction an understanding of the chemical bond helps in predicting the reactivity or properties for the surface system.

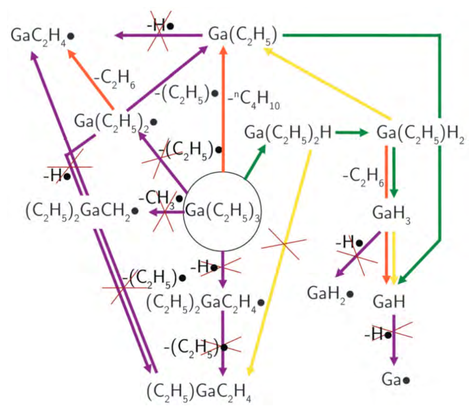
Natural Orbitals for Chemical Valence is an extension to the EDA to visualize changes in the electron denisty in the bond formation. The example shows the electron flow (red to blue) for naphthalene on silicon.



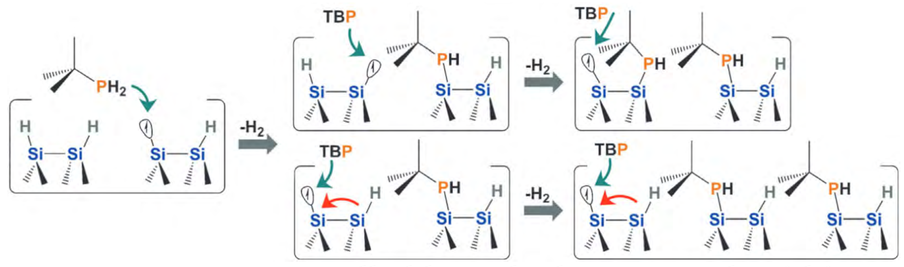
Modelling of Thin Film Growth



Area-selective atomic layer deposition is a promising tool for the production of next generation electronic devices. Here, theoretical models help to understand the elemental reaction steps.



In the chemical vapor deposition the used precursor molecules already decompose in the gas phase. Modelling all possible reaction channels enables to predict the main adsorbing molecules.



For a controlled layer-by-layer growth within the ALD and CVD the surface adsorption and reactivity of all used molecules has to be understood. The example of tert-butylphosphin on silicon shows that this is a nontrivial research question.

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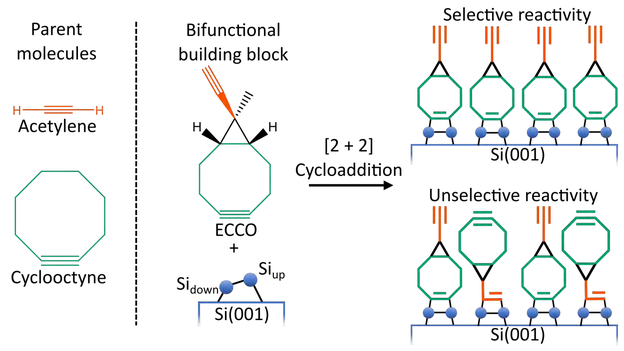
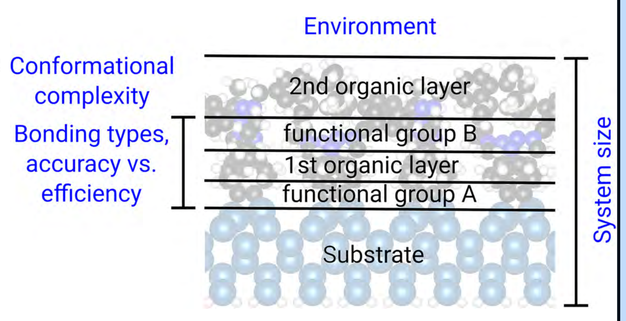
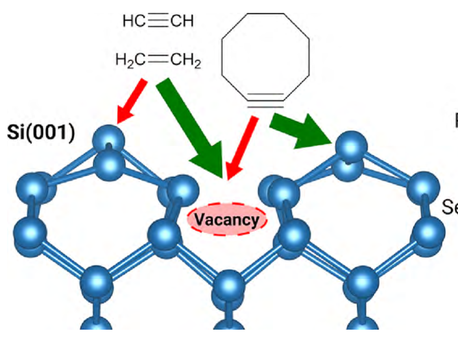
Surface and Interface Chemistry



The formation of organic-inorganic interfaces is a crucial step for the development of molecular electronics. Especially, a controlled formation of the first organic layer is of interest. Therefore, the adsorption of bifunctional cyclooctyne derivates is studied.

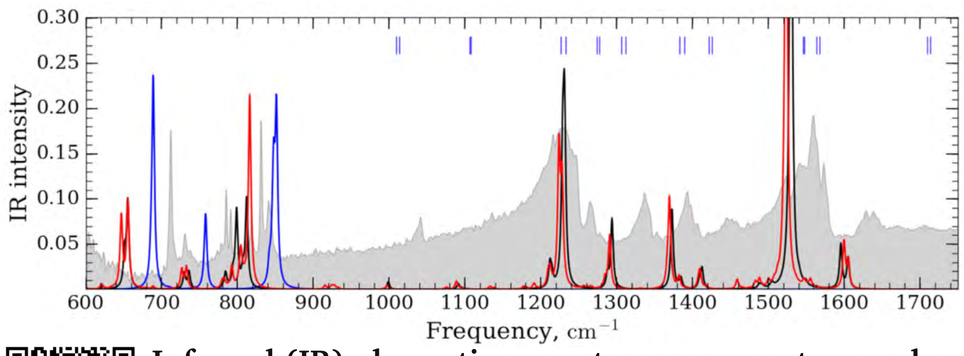
Models dealing with a surface and several organic adsorbates are computationally higly demanding. Consequently, to study the reactivity of the organic layers hierarchical models are used, which incorporate substrate and environmental effects only to a certain degree.



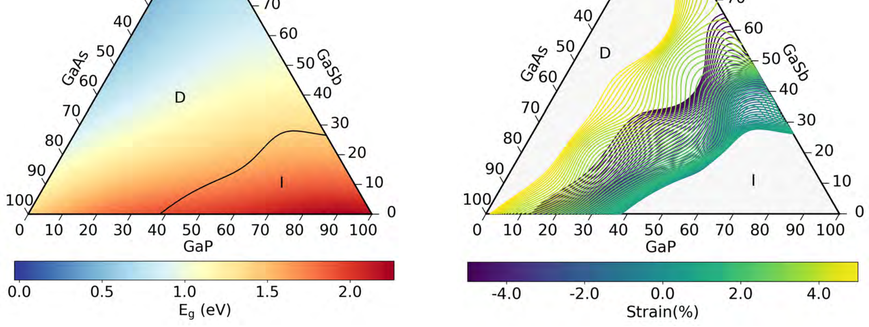


Idealized models are well suited to understand fundamental properties and trends. However, more realistic models are seeked to meet experimental conditions as closely as possible. Surface defects are studied since they can have a large effect on the reactivity of adsorbates.

Understanding Molecular and Electronic Properties



Infrared (IR) absorption spectroscopy spectra can be calculated to refine experimental observations with a structural model. In this example, mono- and bilayers of PTCDA on Ag(111) are investigated.



One of the most prominent electronic property of composite materials is their bandstructure. Here, the bandgap of GaAsPSb is tuned by focusing on the biaxial strain of the material.

Cooperations

Interested in combining theoretical chemistry with your research in other fields?

Take a look at the following publications to get an idea of how cooperations could look like.

Organic Chemistry

Inorganic Chemistry

Physical Chemistry

Chemical Biology

Surface Science

Solid-State Chemistry

Material Sciences