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"Energy-based bonding analysis for surface and material sciences"

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In molecular chemistry, quantum chemical methods reached a state where accuracy is comparable or even exceeds experimental approaches. Similarly, bonding and reactivity concepts based on analysis methods for wave function- or density functional theory-based computations are well established and very often complement experimental studies to aid interpretation or predict new chemistry. Surprisingly, this fruitful interplay of quantitative and qualitative theoretical approaches and experiment has barely been extended to surfaces and solids.[1]
We recently developed a new method for the analysis of chemical bonding and reactivity in periodic systems (pEDA), which now allows the transfer of concepts like donor-acceptor bond, covalency, σ/π-bonding or steric repulsion to periodic systems.[2] We combine this with other electronic structure analysis methods to move from structure (a), to quantitative analysis of bonding contributions (b) to models predicting new reactivity (c). Based on examples from organic functionalization of semiconductors,[3] surface chemistry in heteroepitaxy thin-film growth [4] or analysis of metalorganic interfaces,[5] the strength of the approach will be highlighted.

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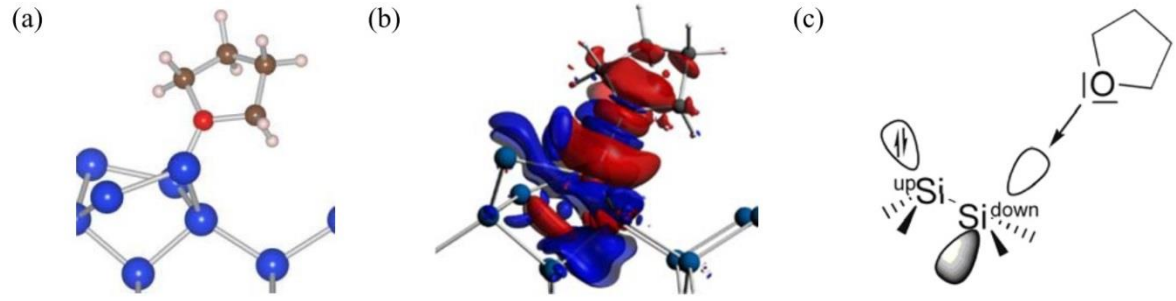

Structure (a), pEDA analysis (b) and bonding model (c) for tetrahydrofurane on Si(001)c(4x2).

[1] a) A. Nilsson, L. G. M. Pettersson, J. Nørskov, Chemical Bonding at Surfaces and Interfaces, Elsevier, Amsterdam, 2007; b) R. Hoffmann, Solids and surfaces, VCH, New York, Weinheim, 1988.
[2] a) M. Raupach, R. Tonner *J. Chem. Phys.* 142 (2015) 194105; b) M. Raupach, T. Ziegler, R. Tonner, in preparation.
[3] G. Mette, M. Reutzel, R. Bartholomäus, S. Laref, R. Tonner, M. Dürr, U. Koert, U. Höfer *Chem. Phys. Chem*. 15 (2014) 3725.
[4] A. Stegmüller, K. Volz, U. Höfer, M. Dürr, R. Tonner et al., to be submitted.
[5] P. Rosenow, P. Jakob, R. Tonner *J. Phys. Chem. Lett*. 7 (2016) 1422.

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