Scientific Computing & Modelling

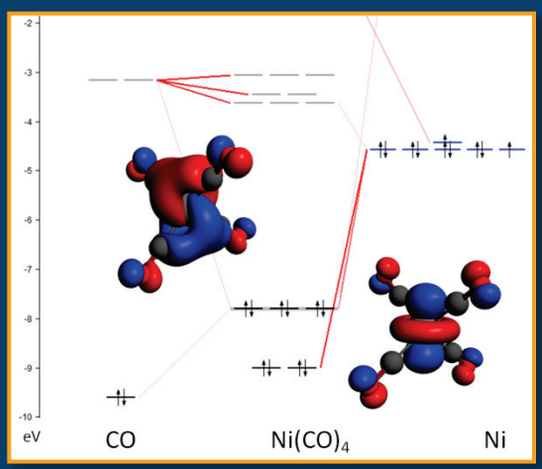
Quality **Software**.
Quantum **Science**.

Analyzing Chemical Bonds with ADF

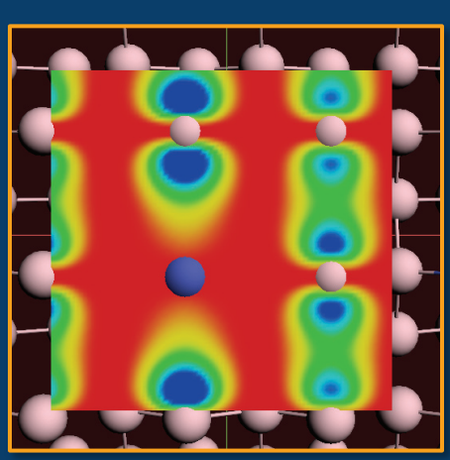
Energy decomposition analysis

- Molecules built from fragments
- Electrostatic & orbital interactions, Pauli repulsion, dispersion
- Detailed orbital interactions: ETS-NOCV

Density and orbital analysis



- Symmetry
- Energy-level diagrams
- Density of states (DOS)
- Partial DOS (pDOS)
- Atoms in Molecules (AIM)
- Natural Bond Order (NBO)
- Non-covalent interactions (NCI)
- Electron-localization function (ELF)
- Single-exponential decay detector (SEDD)
- Bond orders: Nalewajski-Mrozek , Gopinathan-Jug, Mayer
- Charges: Mulliken, Hirshfeld, Voronoi, multipole-derived, AIM
- Quick visualization of various potentials and fields
- STM images (Tersoff-Hamann), band structures, Fermi surfaces
- All-electron Slater orbitals for all elements



General

- Fully integrated graphical interface
- Expert staff and support
- Latest developments, functionals
- Accurate relativistic effects
- Strong in spectroscopy and analysis

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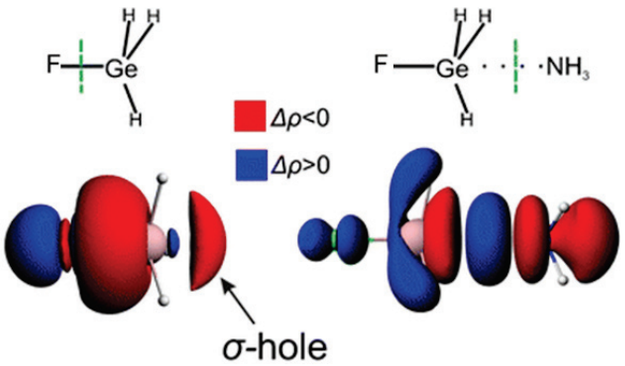
Chemical Bonding Analysis Research Highlights

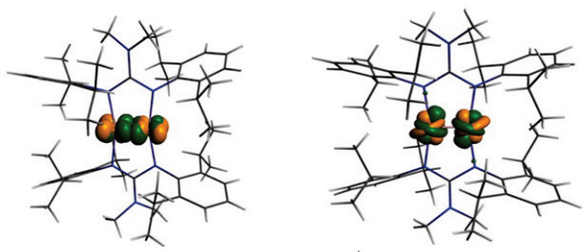
ETS-NOCV analysis of the σ-hole in halogenated compounds and its bonding interaction with ammonia: electrostatic and orbital interactions.



K. Dyduch, M. P. Mitoraj, and A. Michalak, *ETS-NOCV description of σ-hole bonding.* J. Mol. Model. (2012)

ETS-NOCV analysis of shortest quintuple metal–metal bond (Cr–Cr = 1.729 Å) and other supported Cr-Cr bonds.

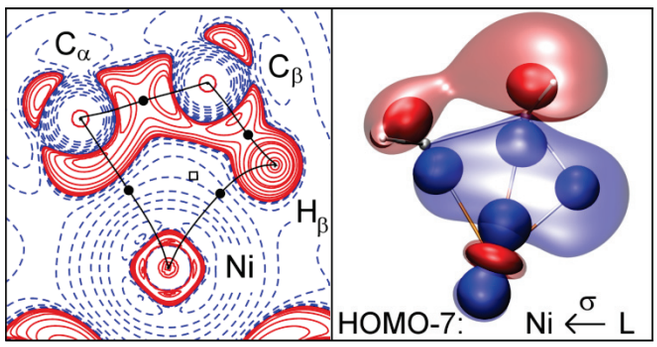
$$\Delta\rho_{orb}^{\pi_1} = \Delta\rho_{orb}^{\pi_1,\alpha} + \Delta\rho_{orb}^{\pi_1,\beta} \qquad \Delta\rho_{orb}^{\delta} = \Delta\rho_{orb}^{\delta,\alpha} + \Delta\rho_{orb}^{\delta,\beta}$$



$$\Delta E_{orb}^{\pi_1} = -60.8\ kcal/mol \qquad \Delta E_{orb}^{\delta} = -40.2\ kcal/mol$$

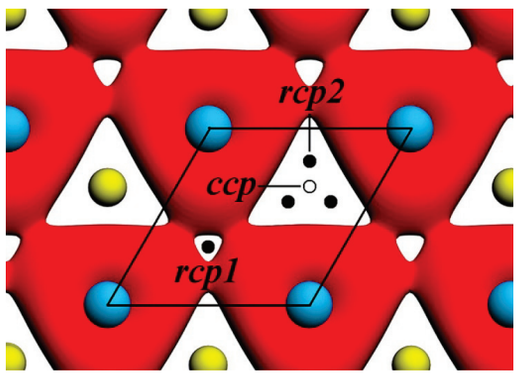
S. Ndambuki and T. Ziegler, *A Theoretical Analysis of Supported Quintuple and Quadruple Chromium–Chromium Bonds.* Inorg. Chem. **52**, 3860 (2013)

Nature of Ni β-agostic bond: charge density analysis and Modified Dewar–Chatt–Duncanson model with 3 σ/π bonds



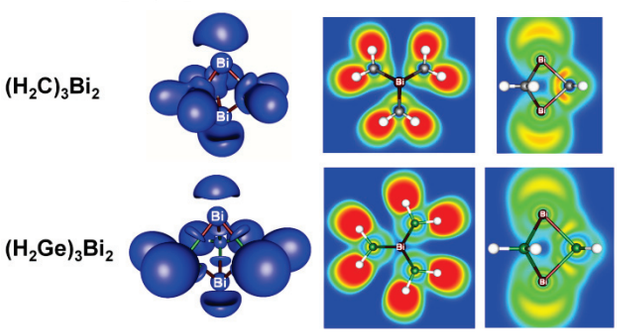
W. Scherer, V. Herz, A. Bruck, C. Hauf, F. Reiner, S. Altmannshofer, D. Leusser, and D. Stalke, *The Nature of β-Agostic Bonding in Late-Transition-Metal Alkyl Complexes.* Angew. Chem. Int. Ed. 50, 285 (**2011**)

Very fast AIM analysis of critical points, also for surfaces (2D)



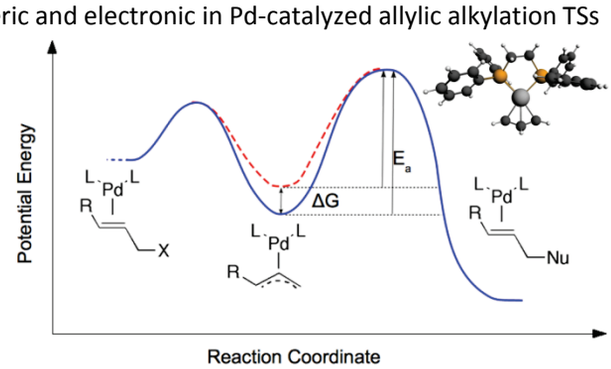
S. P. Gabuda, S. G. Kozlova, M. R. Ryzhikov, and V. E. Fedorov, *Transition from 2-D Semiconductor to 1-D Metal State and Electron Density Distribution in Nanolayered MoX_2 (X = S, Se, Te).* J. Phys. Chem. C **116**, 20651 (2012)

NBO, ELF, and EDA analysis of free and transition-metal complexed $(R_2E)_3Bi_2$ bicyclopentanes



K. Yu. Monakhov and C. Gourlaouen, *On the Insertion of ML2 (M = Ni, Pd, Pt; L = PH3) into the E–Bi Bond (E = C, Si, Ge, Sn, Pb) of a Bicyclo[1.1.1]Pentane Motif: A Case for a Carbenoid-Stabilized Bi(0) Species?* Organometallics **31**, 4415 (2012)

Activation strain analysis bite angle effects: subtle opposing steric and electronic in Pd-catalyzed allylic alkylation TSs



J. Wassenaar, E. Jansen, W.-J. van Zeist, F. M. Bickelhaupt, M. A. Siegler, A. L. Spek, and J. N. H. Reek, *Catalyst selection based on intermediate stability measured by mass spectrometry.* Nature Chem. **2**, 417 (2010)

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