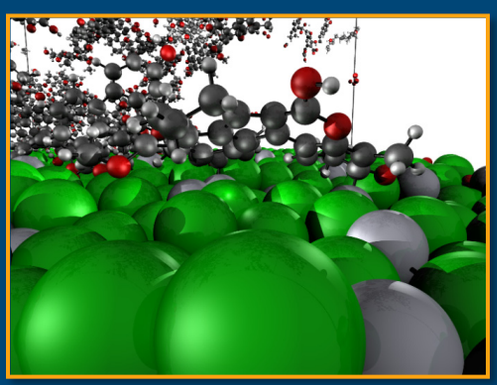
Scientific Computing & Modelling

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

ADF Modeling Suite for Petrochemistry

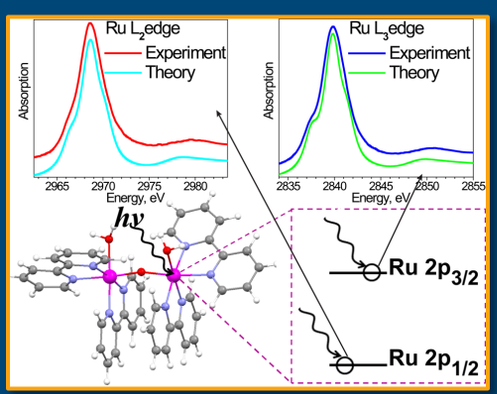
Easy integrated modeling solution

- Atomistic (DFT, DFTB, MOPAC, ReaxFF) & continuum (COSMO-RS)
- Cross-platform (Windows, Linux, Mac)
- Single graphical interface
- Parallel install out of the box
- Expert staff and support



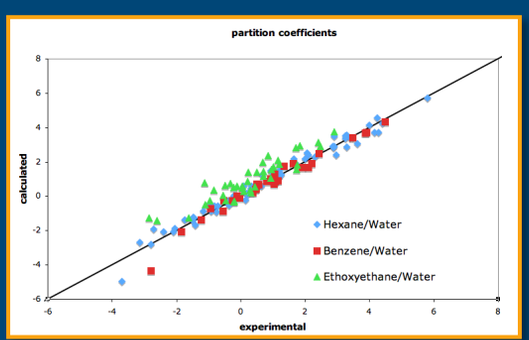
Catalysis

- Surfaces 2D: no dipole issues, solvation
- Molecular + Periodic DFT
- Chemical bond analysis: rational design
- Spectroscopy: XAS, EPR, NMR, UV/VIS
- Strong in transition metal chemistry
- All-electron basis, relativistic effects
- Semi-empirical: MOPAC, DFTB
- Reactive MD: chemistry of large, complex systems



COSMO-RS: fluid thermodynamics

- Quantum-based predictions
- VLE, LLE, logP, solubilities
- COSMO-SAC-2013: improved VLE
- Compounds database



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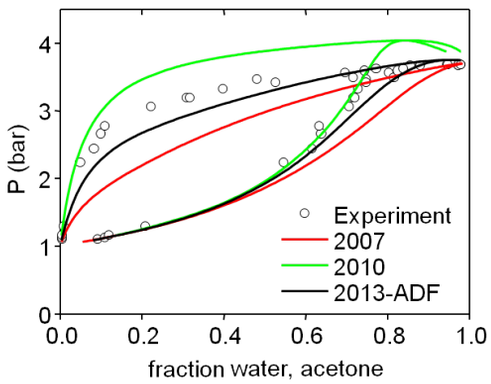
Petrochemistry Modeling Research Highlights

Improved thermodynamic properties with COSMO-SAC-2013



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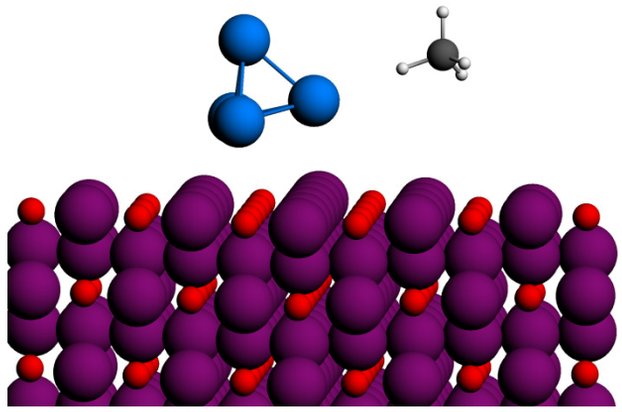
Al_2O_3 support acts as e-donor for methane activation over Ni



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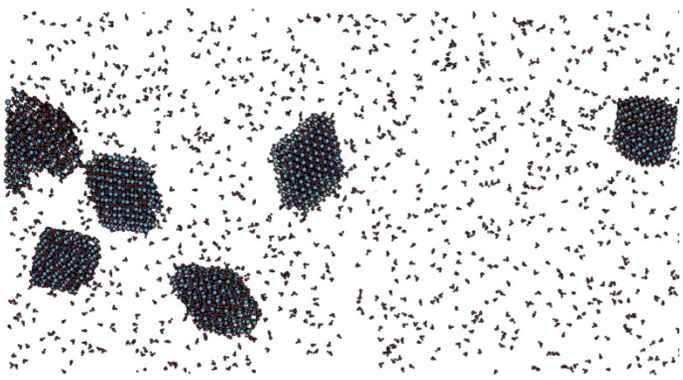
Crystal growth: oriented attachment of TiO_2 nanoparticles



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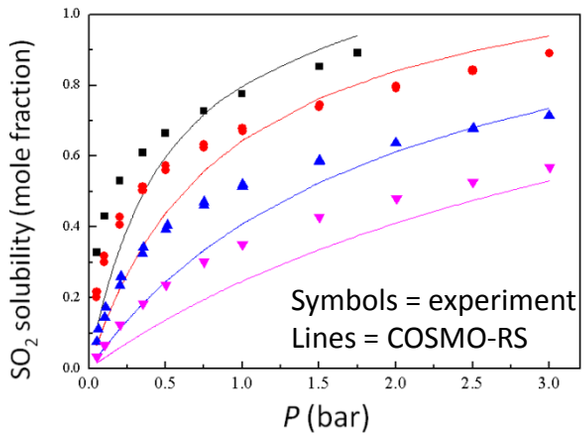
SO_2 solubility in $[BMIM]^+[MeSO_4]^-$ with COSMO-RS



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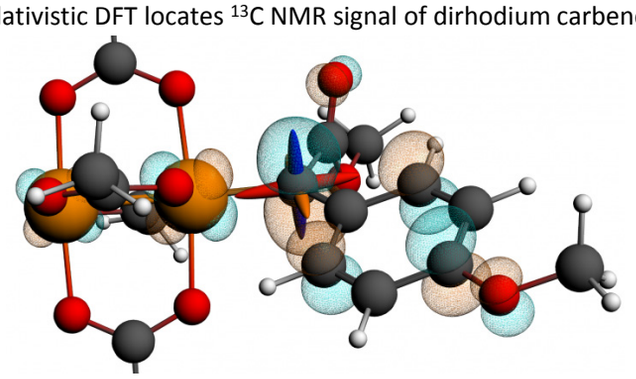
Relativistic DFT locates ^{13}C NMR signal of dirhodium carbene



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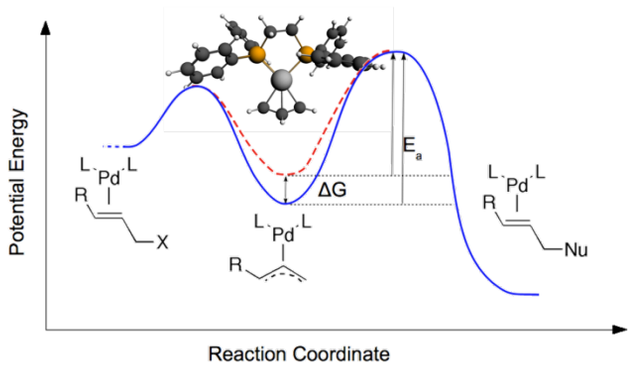
Survival of the weakest, catalyst design by bonding analysis



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