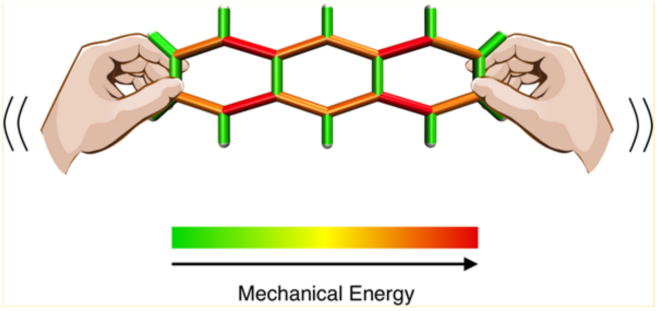
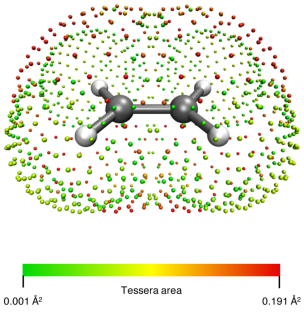
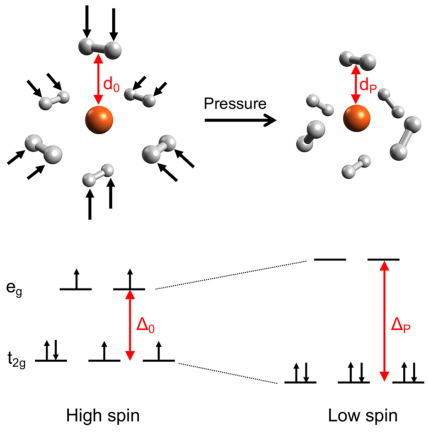
Q-CHEM™
A Quantum Leap Into the Future of Chemistry

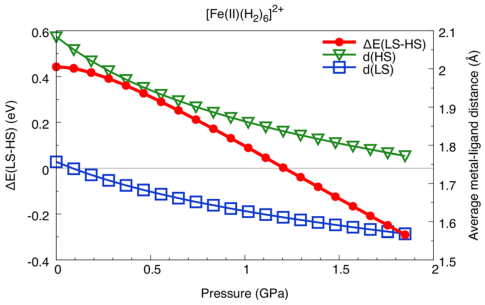
Quantum Mechanochemistry: Molecules under External Forces





- Mechanochemistry studies the coupling of mechanical and chemical phenomena on a molecular scale. It reveals the relation between external forces and molecular properties or chemical reactivity.
- Q-Chem enables modeling molecular electronic structure under external pressures. Three theoretical models are available: Hydrostatic Compression Force Field (HCFF), extended Hydrostatic Compression Force Field (X-HCFF), and Gaussians On Surface Tesserae Simulate HYdrostatic Pressure (GOST-SHYP). They are available in geometry optimization and AIMD calculations.
- The quantum mechanochemistry methods can find applications in single-molecule force spectroscopy (SMFS), sonochemistry (chemistry caused by ultrasound), nanoparticle synthesis and molecular machine design.





High hydrostatic pressure in $(Fe(II)(H_2)_6)^{2+}$ leads to a switching of the high spin state to the low spin state

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