Theory and modeling of 2D materials

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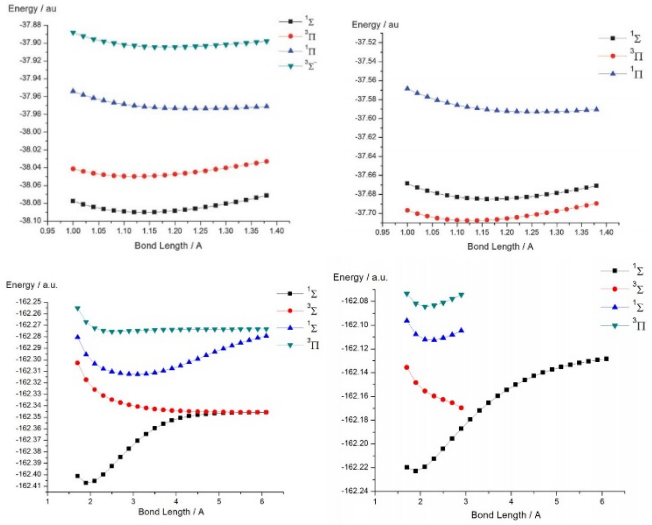

***Upper*:** pp-RPA (left) and TD-LDA (right) results for the ground state and excited states for the CH^+ molecule
Middle: pp-RPA (left) and TD-LDA (right) results for the ground state and excited states for the NaH molecule

Keys features

- Density Functional Theory
- Linear scaling and multiscale approaches
- Design of molecules/materials

Scope of effort

- Modeling of the reaction mechanisms and transport in 2D materials
- Describing excitations and double-excitations with particle-particle random phase approximations (pp-RPA)
- Developing embedding approaches for modeling excitations in 2D and 3D materials with pp-RPA
- Incorporating new functionals in linear scaling approach for large systems

Challenges to address

- The structure characterization of molecules on 2D materials, the nature and effects of defects
- Description of extended systems with pp-RPA