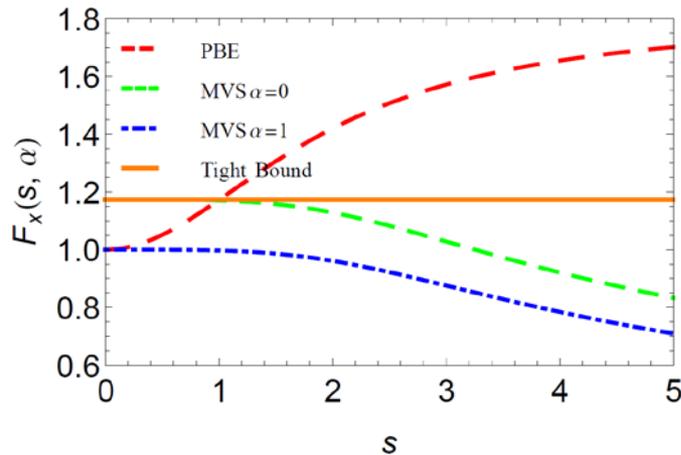


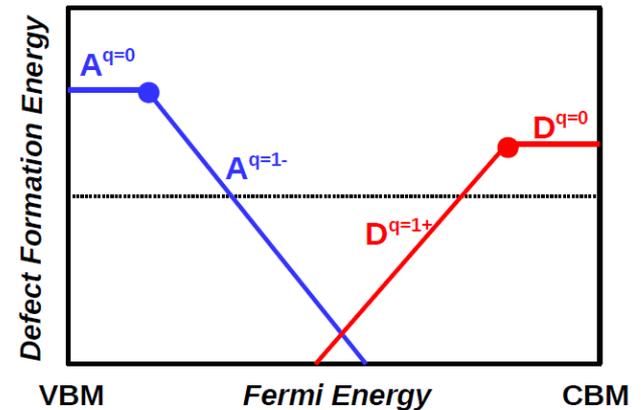
Defect engineering of 2D materials



Jianwei Sun



The MVS MGGA respects an exact constraint, the tight bound on the exchange energy that PBE violates



Schematic representations of defect formation energy and transition energy levels of different charge states of a donor and an acceptor.

Scope of effort

- Development of new density functionals
- Testing density functionals for 2D materials and 3D layered materials
- Defect engineering of 2D materials computationally

Challenges to address

- Development of an efficient nonempirical universal density functional for vdW-bound layered materials that usually involve d- and f-electrons
- Accurate calculations of defect formation energy and transition energy level for 2D materials
- Understanding nature and the impact of defects and its usage for tailoring new 2D materials