# Density Functional Theory of Materials

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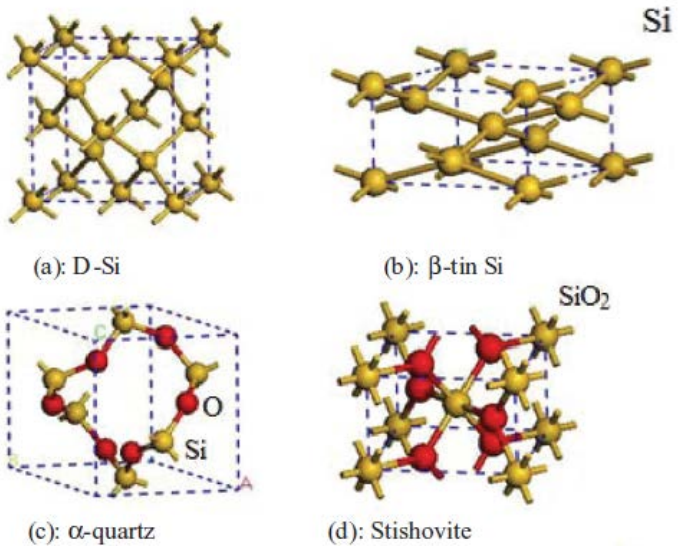


The crystal structures of silicon and silicon dioxide polymorphs can be predicted by theory.

## Key feature

- For computational searches over many candidate materials, we need efficient but accurate and widely-applicable density functionals for the exchange-correlation energy of the electrons.

## Scope of effort

- With NSF support, develop an improved meta-generalized gradient approximation (meta-GGA) that recognizes and appropriately treats covalent, metallic, and weak bonds. With DOE support, apply this meta-GGA, with or without fully-nonlocal corrections, to the pristine and defected layered materials.

## Challenges to address

- Satisfy all possible exact constraints on the meta-GGA. Then develop or test ways to include long-range van der Waals and self-interaction corrections, as needed.