# Testing density functionals for structural phase transitions of solids under pressure: Si, SiO2, and Zr

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## Abstract

We have investigated the structural phase transitions of crystalline Si (insulator-metal), SiO2 (insulator-insulator), and Zr (metal-metal) under pressure, as a test of several density functionals for the exchange-correlation energy. While meta-generalized gradient approximations (meta-GGAs) such as revTPSS (revised Tao-Perdew-Staroverov-Scuseria) are more sophisticated than GGAs such as PBE (Perdew-Burke-Ernzerhof), and are more accurate without empiricism for atomization energies of molecules, lattice constants of solids, and surface energies, we confirm that these meta-GGAs tend to give smaller and less realistic transition pressures than the PBE GGA does. But we also show that the recent functionals of the meta-GGA made simple family (MGGA_MS) behave differently, predicting larger and often more realistic transition pressures. We suggest that further refinement of the meta-GGA can lead to a functional that is more accurate for properties of molecules and solids at equilibrium or under compression. We also show that, contrary to recent suggestions but in line with older ones, an accurate fundamental gap in the noninteracting band structure is not necessary for an accurate prediction of the transition pressure. Unlike the semilocal GGAs and meta-GGAs, and unlike the local density approximation also tested here, the screened hybrid functional HSE06 (Heyd-Scuseria-Ernzerhof) is fully nonlocal and predicts more realistic fundamental gaps. HSE06 is better than the semilocal functionals for the transition pressures of Si and SiO2, but seriously overestimates the transition pressure in Zr. Besides the transition pressures, we report the transition energies and volumes, binding energy curves, and structural parameters at zero and transition pressure. Finally, we discuss how the performance of a functional can reflect its plottable exchange enhancement factor, and why the structural phase transitions are especially challenging for approximate density functionals.

## Keywords

**KeyWords Plus:** GENERALIZED-GRADIENT-APPROXIMATION; EXCHANGE-CORRELATION ENERGY; ELECTRONIC-STRUCTURE; ALPHA-QUARTZ; SPIN-DENSITY; AB-INITIO; STISHOVITE; STATE; SILICA; MODEL

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