Proton behaviour, structure and elasticity of serpentine at high-pressure

MAINAK MOOKHERJEE, Yale University, LARS STIXRUDE, University of Michigan — Serpentine occurs in oceanic crust as the alteration product of ultramafic rocks and is a possible candidate for carrying water to the deep earth. The presence of sub-surface serpentine may be manifested by mud volcanoes, high electrical conductivities, and seismic anomalies. Using density functional theory, we predict a phase transition in serpentine near 22 GPa. The phase transition is caused by a re-orientation of the hydroxyl vector coupled with changes in the di-trigonal rings of SiO$_4$ tetrahedra. The symmetry of the crystal-structure remains unaffected. Evidence of pressure-induced hydrogen bonding is absent in serpentine, as evident from the reduction of O-H bond length upon compression. Results of compression for the low-pressure phase is well represented by a fourth order Birch-Murnaghan finite strain expression with $K_O = 63$ GPa, $K_O' = 10.2$ and $K_O K_O'' = -120$, where $K$ is the bulk modulus, prime indicates pressure derivatives, and O refers to zero pressure. At low pressures, the elastic constant tensor is highly anisotropic with $C_{11}^O \sim 2.4 \times C_{33}^O$, and becomes more isotropic with compression. We find an elastic instability near 36 GPa that may be related to experimentally observed amorphization.