Calculations of electronic structure and chemical bonding of stishovite

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Electronic state calculations of stishovite, one of the high pressure polymorphs of SiO2, were carried out in order to investigate the nature of chemical bonding. Based on Bader's theory, mapping of laplacian of electron density distributions enables to reveal the accumulation of bonding electrons in interatomic region. Our result indicate that the covalency of Si-O bonds of stishovite increase with pressure.

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