Abstract Submitted
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Ab initio study of properties of $BaBiO_3$ at high pressure[1] ROMAN MARTOŇÁK, Comenius University in Bratislava, Slovakia, DAVIDE CERESOLI, ISTM-CNR, Università Milano, Italy, TOMOKO KAGAYAMA, Kyokugen, Osaka University, Japan, ERIO TOSATTI, SISSA and ICTP Trieste, Italy — $BaBiO_3$ is a mixed-valence perovskite which escapes metallic state by creating a Bi-O bond disproportionation or CDW pattern, resulting in a Peierls semiconductor with gap of nearly 1 eV at zero pressure. Evolution of structural and electronic properties at high pressure is, however, largely unknown. Pressure, it might be natural to expect, could reduce the bond-disproportionation and bring the system closer to metalicity or even superconductivity. We address this question by ab initio DFT methods based on GGA and hybrid functionals in combination with crystal structure prediction techniques based on genetic algorithms. We analyze the pressure evolution of bond disproportionation as well as other order parameters related to octahedra rotation for various phases in connection with corresponding evolution of the electronic structure. Results indicate that $BaBiO_3$ continues to resist metalization also under pressure, through structural phase transitions which sustain and in fact increase the diversity of length of Bi-O bonds for neighboring Bi ions, in agreement with preliminary high pressure resistivity data.

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