

# Ab-initio Studies of Pressure Induced Phase Transitions in BaO

M. Uludođan<sup>1</sup>, T. ađın<sup>2</sup>, A. Strachan<sup>2</sup> and W. A. Goddard III.<sup>2</sup>

<sup>1</sup> Department of Physics, Middle East Technical University, 06531 Ankara, TURKEY

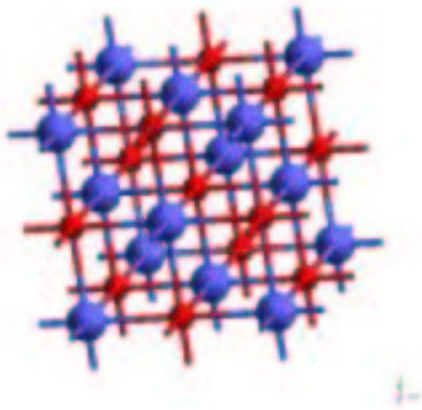
<sup>2</sup> Materials and Process Simulation Center, Beckman Institute (139-74) California Institute of Technology, Pasadena, California 91125

Due to their geophysical importance, earth oxides are studied extensively. Their high pressure behavior and phase transformation are explored both experimentally and theoretically. In this work, we will present first principles calculations (purely quantum mechanics- no empirical parameters) study on the phase diagram of BaO. We studied the equation of state of BaO in B1(NaCl), B8(NiAs), B2(CsCl) and distorted B2 phases of BaO. We employed density functional theory with the generalized gradient approximation to obtain the equation of state for these phases over a wide range of pressures. We have elucidated the phase transformations observed between these phases (Table.1). As it is well known, at very high pressure almost all materials go through a metallization transition. We also studied this for BaO.

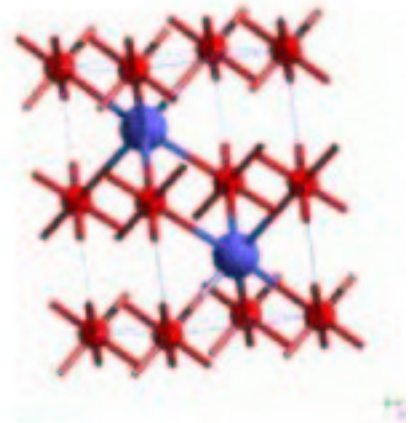
Table 1: Experimental and theoretical phase transitions from B1 phase to B8 phase, from B8 phase to distorted B2 phase and from distorted B2 phase to B2 phase. Theoretical results are 0 K results, and the experimental results are room temperature results.

Phase Transition	B1 to B8 (GPa)	B8 to Dist. B2 (GPa)	Dist.B2 to B2 (GPa)
Lin-Gun Liu et. al., (1972)	9.2	18.0	
Samuel T. Weir et. al., (1986)	9.2	14.0	
Theory (This Work)	11.3	21.5	62.1

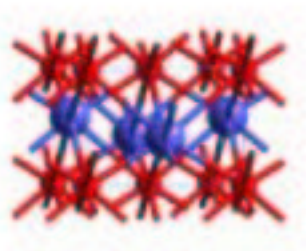
B1



NiAs(B8)



Distorted B2



B2

