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Effect of temperature and pressure on molar volume of ZnO Wurtzite phase under extended pressure and temperature a molecular dynamics prediction

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The behavior of molar volume of ZnO wurtzite phase is investigated using parallel molecular dynamics and dl_poly_4 software in RAVEN supercomputer of Cardiff University (UK). In this work we study the effect of temperature and pressure on molar volume of ZnO wurtzite type in the range of 300-3000K and 0-200GPa of temperature and pressure respectively. We analyze the relationship between pressure and temperature on molar volume; our data are in agreement with available results, although no more work under the previous conditions of pressure and temperature. Our work is very important in medicine, pharmacy, and geophysics, which need confirmation in future.

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