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Phonon dispersions and structural transitions of CrO_2 under high pressure SOORAN KIM, KYOO KIM, CHANG-JONG KANG, B.I. MIN, POSTECH — Phonon dispersions of chromium dioxide (CrO_2) are calculated to investigate the structural phase transitions as a function of pressure. The structural phase transition has been confirmed from the ground state tetragonal CrO_2 of rutile-type (t-CrO_2) to the orthorhombic CrO_2 of $CaCl_2$-type (o-CrO_2). The ferromagnetic and half-metallic property is preserved even in o-CrO_2. The softening of Raman-active B_{1g} phonon mode, which is relevant to the above structural transition, is also obtained. We will discuss the possible more structural phase transitions from o-CrO_2 and the related phonon and magnetic properties at much higher pressure.

[X] Prefer Oral Session
[ ] Prefer Poster Session

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