Abstract Submitted
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An Investigation of s-d promotion at high pressure with the Projector Augmented Wave method[1] RYAN SNOW, University of California, Davis, JOHN PASK, Lawrence Livermore National Laboratory, CHING-YAO FONG, University of California, Davis — The PAW(1) method for ab initio density functional calculations combines advantages of both pseudopotential (PP) and all-electron (AE) methods. The PAW method provides accuracy comparable to AE methods, core-sensitive calculations, and ab initio molecular dynamics with large systems. The requirement for high accuracy in the determination of s-d promotion pressures in transition metals serves as a proving ground for the accuracy of the PAW method. We present PAW, PP, and AE APW+lo results for the case of Molybdenum, for which there is significant disagreement among recent ab initio predictions above 600 GPa. 1. P.E. Blochl, Physical Review B, 50, 17953 (1994)

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