Accuracy and limitations of some projector augmented wave pseudopotentials for metals at high pressures

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The method of projector augmented wave (PAW) pseudopotentials is widely used [1] to investigate properties of metals at extreme conditions, particularly high pressures. In this work, we study pseudopotentials presented in Vienna Ab initio Simulation Package [2] (VASP) in a wide range of pressures. Our research is dedicated to *ab initio* calculations of cold curves for several metals: Ag, Mo, Ti, Cu, Na, Mg, Zr, Rb, and Fe. Different crystal structures are considered for metals with polymorphic phase transitions. Additionally, the impact of the magnetic moment for Fe is studied. The limitations of pseudopotentials are analyzed by comparing with more accurate potentials. We also present the comparison of the calculated cold curves for different pseudopotentials with available diamond anvil cell experimental data. The work has been supported by the Russian Science Foundation (grant No. 20-79-10398).

[1] Kresse G and Joubert D 1999 *Phys. Rev. B* **59** 1758–1775
[2] Kresse G and Furthmüller J 1996 *Phys. Rev. B* **54** 11169