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Comparison for Some Elastic and Mechanical Properties of Plutonium Dioxide

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Abstract: We report some elastic parameters of cubic fluorite type neptunium dioxide (NpO2) with a recent EAM type interatomic potential through geometry optimization calculations. Typical cubic elastic constants, bulk modulus, shear modulus, young modulus and other relevant elastic parameters were also calculated during research. After calculations, we have compared our results with the available theoretical data. Our results agree well with the previous theoretical findings of the considered quantities of NpO2.

Keywords: NpO2, elastic properties, bulk modulus, mechanical properties

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