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Pressure-induced core-level crossing transitions in 5d metals.[1]
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Considering hexagonal closed-packed Os compressed to over 770 GPa, we discuss the anomaly observed experimentally in the behavior of the unit cells parameters ratio c/a at about 440 GPa. We argue that the anomaly is related to a new type of electronic transition, the core level crossing (CLC) transition, associated with interactions between the core electrons induced by pressure [1]. By carrying out a systematic theoretical study for all metals of the 5d series (Hf, Ta, W, Re, Os, Ir, Pt, Au) we have found that the CLC transition is a general effect for this series of metals. While in Pt it occurs at ≈1500 GPa, at a pressure substantially higher than in Os, in Ir it occurs already at 80 GPa. Moreover, we predict that in Re the CLC transition may take place already at ambient pressure. We explain the effect of the CLC and analyze the shift of the transition pressure across the series within the Thomas-Fermi model. In particular, we show that the effect has many common features with the atomic collapse in rare-earth elements [2]. [1] L. Dubrovinsky *et al.*, Nature 525, 226–229 (2015). [2] A. A Tal *et al.*, Phys. Rev. B 93, 205150 (2016).

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