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Influence of van der Waals corrected *xc*-functionals on the anisotropic mechanical properties of coinage metals JI-HWAN LEE, JONG-HUN PARK, YOUNG-KWANG JUNG, ALOYSIUS SOON, Global E3 Institute and the Department of Materials Science and Engineering, Yonsei University, Seoul 121-749, South Korea — Current materials-related calculations employ the density-functional theory (DFT), commonly using the (semi-)local-density approximations for the exchange-correlation (*xc*) functional. The accuracy to studying the electronic structure depends not only on the employed approximation to the *xc* potential but also upon the system which is being investigated. The difficulties in arriving at a reasonable description of van der Waals (vdW) interactions by DFT-based models, is to date a big challenge. This stems from the well-known fact that vdW interaction is a non-local correlation effect which is not captured in the deployed (semi-)local *xc* functionals. In this work, using various flavours of vdW-corrected DFT *xc* functionals, we study the lattice and mechanical properties (including the elastic constants and anisotropic stress-strain curves) of the coinage metals (copper, silver, and gold), and critically assess the reliability of the different vdW-corrected DFT methods in describing their anisotropic mechanical properties which are less reported on in the literature.

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