Erratum: Vibrational Frequencies of Cerium-Oxide-Bound CO: A Challenge for Conventional DFT Methods [Phys. Rev. Lett. **125**, 256101 (2020)]

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In this Letter, Fig. 2(c) mistakenly shows the HSE06 isosurface of the charge density difference instead of that obtained with PBE + U .

The authors state that the mistake does not change the scientific conclusions of the article in any way since the discussion in the text, as published, is correct.

FIG. 2. Total density of states (DOS) projected onto the CO (blue) for 1 ML CO adsorbed on the CeO₂(111) surface in the atop Ce⁴⁺ configuration with the (a) PBE + U (4.5) and (b) HSE06 approaches compared to that of CO in the gas phase. (c),(d) Isosurfaces of the charge density difference, namely, that of the CO adsorbed system from which both the charge density of the clean CeO₂(111) surface (with a structure corresponding to that of the adsorbed system) and that of the layer of adsorbed CO molecules have been subtracted. Selected interatomic distances (in pm) are indicated.