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**Orbital Delocalization and Enhancement of Magnetic Interactions in Perovskite Oxyhydrides** KAI LIU, YUSHENG HOU, XINGAO GONG, HONGJUN XIANG, Fudan University, CCMG TEAM — Recent experiments showed that some perovskite oxyhydrides have surprisingly high magnetic-transition temperature. In order to unveil the origin of this interesting phenomenon, we investigate the magnetism in SrCrO<sub>2</sub>H and SrVO<sub>2</sub>H on the basis of first-principles calculations and Monte Carlo simulations. Our work indicates that the Cr-O-Cr superexchange interaction in SrCrO<sub>2</sub>H is unexpectedly strong. Different from the previous explanation in terms of the H<sup>-</sup> ion substitution induced increase of the Cr-O-Cr bond angle, we reveal instead that this is mainly because the 3*d* orbitals in perovskite oxyhydrides becomes more delocalized since H<sup>-</sup> ions have weaker electronegativity and less electrons than O<sup>2-</sup> ions. The delocalized 3*d* orbitals result in stronger Cr-O interactions and enhance the magnetic-transition temperature. This novel mechanism is also applicable to the case of SrVO<sub>2</sub>H. Furthermore, we predict that SrFeO<sub>2</sub>H will have unprecedented high Neel temperature because of the extraordinarily strong Fe-H-Fe  $\sigma$ -type interactions. Our work suggests the anion substitution can be used to effectively manipulate the magnetic properties of perovskite compounds.

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