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【617】 Metal-insulator transition in CaVO_3 thin films from DFT+DMFT

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Complex oxide thin films and heterostructures exhibit a wide variety of interesting functionalities that are generally determined by numerous factors.

Here, we investigate the effects of epitaxial strain, dimensional confinement, as well as interface and surface effects on the electronic properties of the correlated metal CaVO_3 , using a combination of density functional theory (DFT) and dynamical mean-field theory (DMFT). We show that tensile epitaxial strain can induce a metal-insulator transition in CaVO_3 , and we demonstrate that this strain effect cooperates with a similar tendency originating from the finite thickness of the film, consistent with recent experimental observations. Furthermore, we also address the influence of the substrate-film interface in $\text{CaVO}_3/\text{LaAlO}_3$ heterostructures.

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