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First principles study of HfV_2 and ZrV_2 phases: Structural analysis and site preference of Cd and Ta dopants

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We present first principles calculations of the electric field gradients (EFGs) in the pure cubic, tetragonal and orthorhombic phases of HfV_2 and in the cubic phase of ZrV_2. Band structure calculations of orthorhombic and tetragonal HfV_2 are presented for the first time. EFGs are also calculated on the inserted Ta and Cd probe atoms, and results are compared with the existing experimental data from time differential perturbed angular correlations and nuclear magnetic resonance measurements. By this comparison, it was possible to determine the exact space group and crystallographic positions of orthorhombic HfV_2, and the site preferences of the Ta and Cd probe atoms. We have also confirmed that the measured nonzero EFG in the Ta-doped cubic HfV_2 structure originates from the displacement of Ta atoms from their equilibrium positions in the cubic environment.