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Theoretical search for new permanent magnets with no rare earth atoms LIQIN KE, VLADIMIR ANTROPOV, Ames Laboratory, MARK VAN SCHILFGAARDE, King's College, London, UK — We use the density functional theory and Quasiparticle Self-Consistent GW approximation to investigate the crystal and electronic structure, magnetic moment, anisotropy, and exchange coupling of $Fe_{16}N_2$, $Fe_{13}Al_3$, Co_7Hf and Zr_2Co_{11}. Both methods show similar results for magnetization and electronic structure. The experimentally unknown crystal structures of Co_7Hf and Zr_2Co_{11} are obtained using structural optimization. We also discuss possible usage of these materials as permanent magnets.

[X] Prefer Oral Session
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