Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

DFT study of magnetic interfaces based on half-metallic $Co_2FeGe_{1/2}Ga_{1/2}$ with *h*-BN and $MoSe_2$ monolayers

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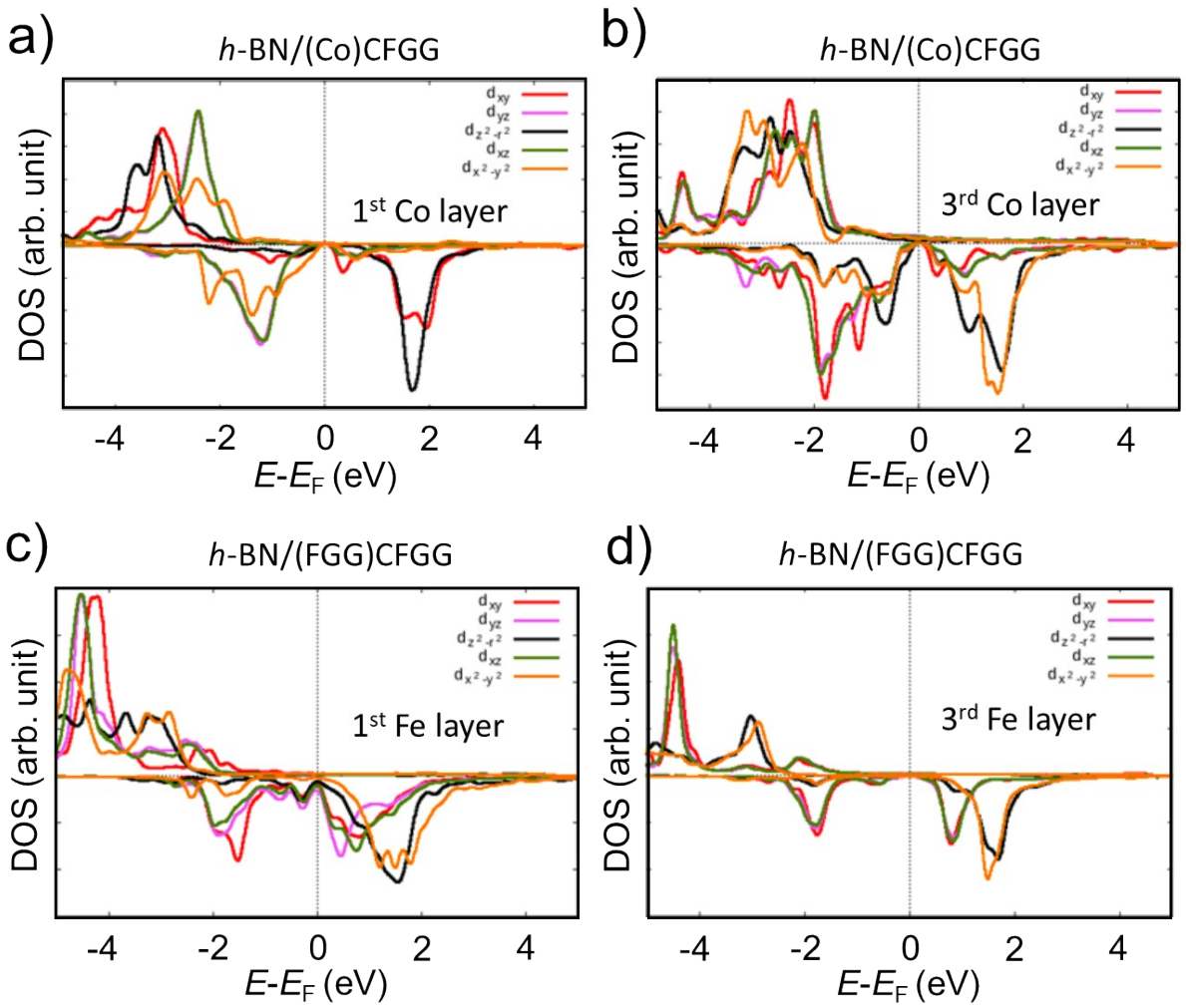

Figure S1. Orbital resolved DOS of Co atoms in (a) the first and (b) the third CFGG layer of Co-terminated *h*-BN/CFGG heterostructure. Orbital resolved DOS of Fe atoms in (c) the first and (d) the third CFGG layer of FGG-terminated *h*-BN/CFGG heterostructure.

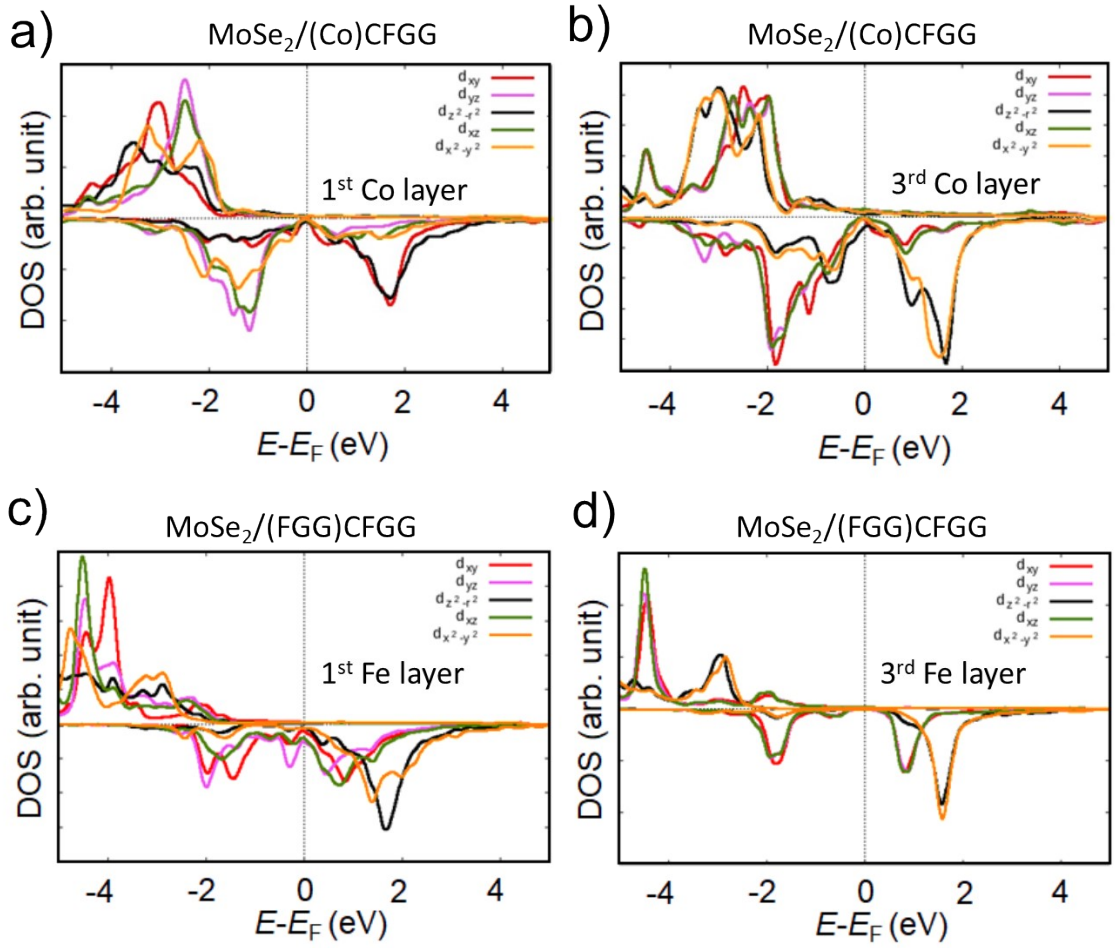

Figure S2. Orbital resolved DOS of Co atoms in (a) the first and (b) the third CFGG layer of Co-terminated $MoSe_2$/CFGG heterostructure. Orbital resolved DOS of Fe atoms in (c) the first and (d) the third CFGG layer of FGG-terminated $MoSe_2$/CFGG heterostructure.

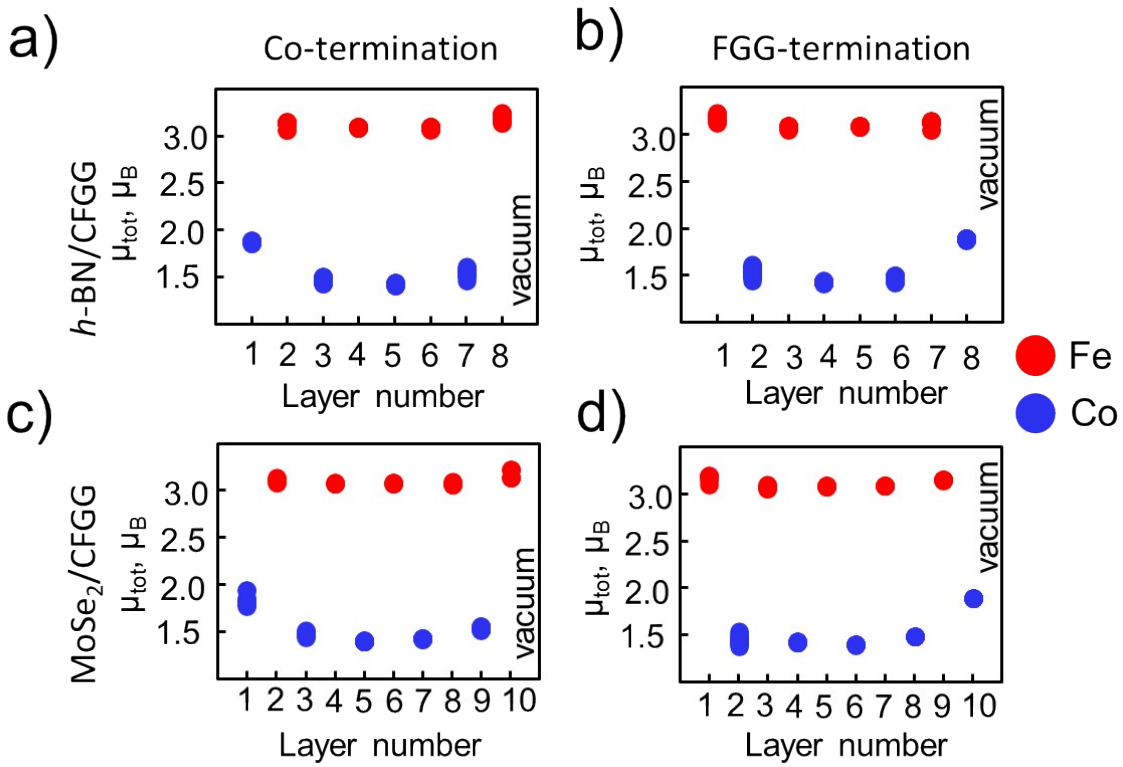

Figure S3. Layer-resolved magnetic moments for Fe and Co atoms in (a,c) Co- and (b,d) FGG-terminated CFGG substrate. Up and bottom row correspond to the *h*-BN/CFGG and $MoSe_2$/CFGG heterostructures, respectively. Red and blue circles denote magnetic moments of iron and cobalt atoms, respectively. CFGG atomic layers are arranged from the top layer nearby interface (1) to the bottom layer nearby vacuum (8 or 10).