

**The EXCHANGE INTERACTIONS DEFINED FINE DETAILS of ATOMIC STRUCTURE of
CrI₃/g-C₃N₄ VERTICAL HETEROSTRUCTURES for PERSPECTIVE SPIN-POLARIZED
PHOTOVOLTAICS**

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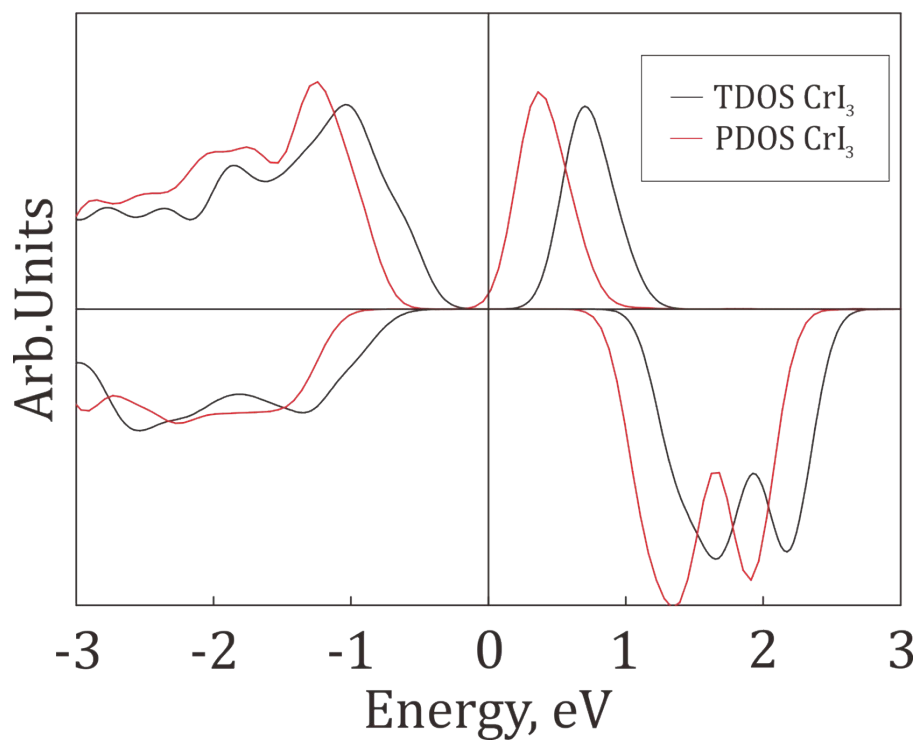


Figure S1. The TDOS of free-standing CrI₃ (black), the PDOS of CrI₃ fragment (red) as a part of CrI₃/g-CN₂/CrI₃ FM heterostructure.

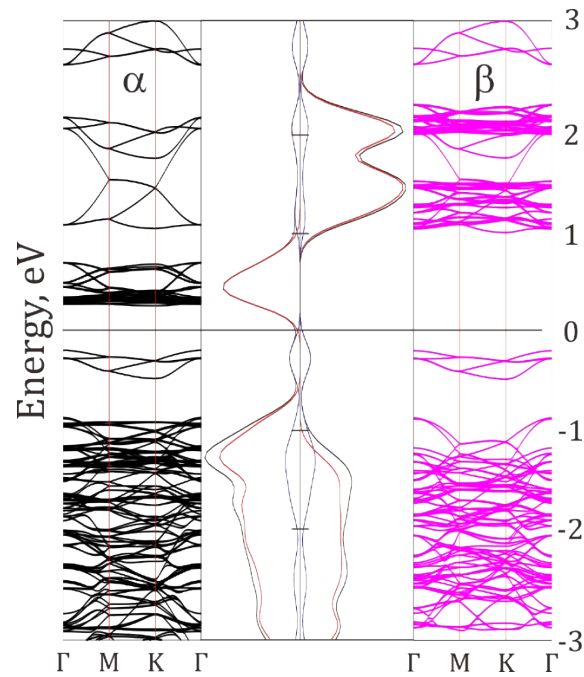


Figure S2. The $\text{CrI}_3/\text{g-CN}_2/\text{CrI}_3$ FM densities of states (middle) and band structure for spin up (right panel) and spin down (left panel) channels. Total DOS is depicted in black, partial DOS of CrI_3 is depicted in red, partial DOS of g-CN_2 is depicted in blue.

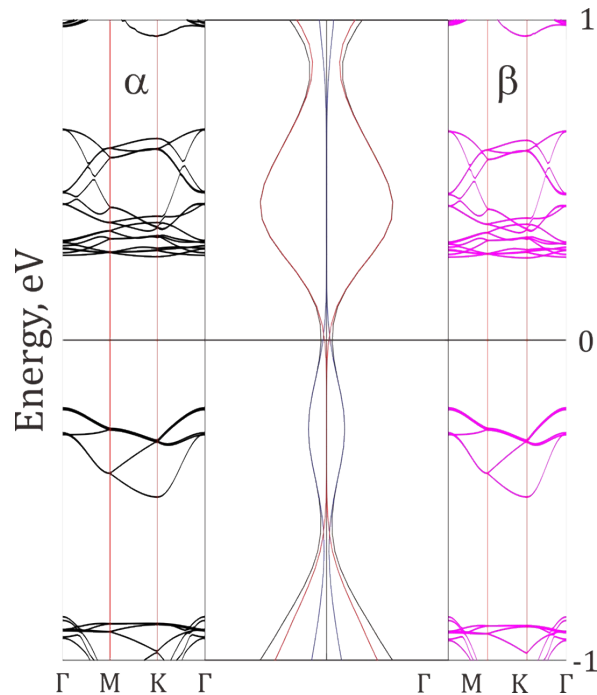


Figure S3. The $\text{CrI}_3/\text{g-CN}_2/\text{CrI}_3$ AFM densities of states distribution (DOS) (middle) and band structure for spin up (right panel) and spin down (left panel) channels. Total DOS are depicted in black, partial DOS of CrI_3 are depicted in red, partial DOS of g-CN_2 are depicted in blue