Theoretical investigation of the magnetic semiconductor nature in PbI_2 monolayer induced by Fe doping

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Table SI: Computational details.

TAG IN INCAR FILE	MEANING
ALGO = FAST	Mixture of the blocked-Davidson and RMM-DIIS algorithms
POTIM = 0.5	Step width in ionic relaxations
PREC = ACCURATE	Precision for the calculations
ISMEAR = 0	Gaussian smearing
SIGMA = 0.05	The width of smearing (eV)
LREAL = AUTO	Projection operators evaluated in real space
LREAL = .FALSE.	Projection operators evaluated in reciprocal space (Only for calculations of magnetic anisotropy energy)
LASPH = .TRUE.	Using non-spherical corrections
ADDGRID = DEFAULT	No additional support grid is used
SYMPREC = 1.0E-8	Accuracy the positions in POSCAR file
QPOINTS	8x8x1 (for supercell 4x4x1)
IBRION = 6	Finite displacement for phonon calculations
IVDW = 11	DFT-D3 method of Grimme with zero-damping function

Table S2. Magnetic anisotropy energy (μeV) of 1Fe@PbI_2 monolayer system calculated with different supercell sizes.

Supercell	MAE
2x2x1	-392.88
3x3x1	-369.95
4x4x1	-353.23
5x5x1	-344.99

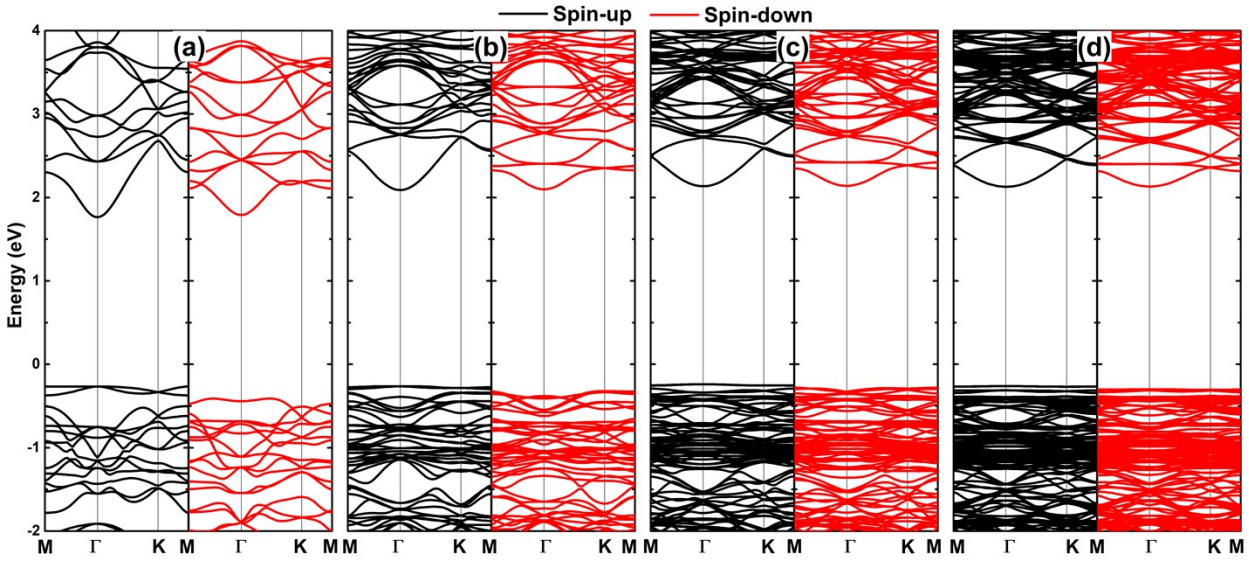

Figure S1: Spin-resolved band structure of 1Fe@PbI_2 monolayer system calculated with (a) 2x2x1, (b) 3x3x1, (c) 4x4x1, and (d) 5x5x1 supercell (The Fermi level is set to 0 eV).

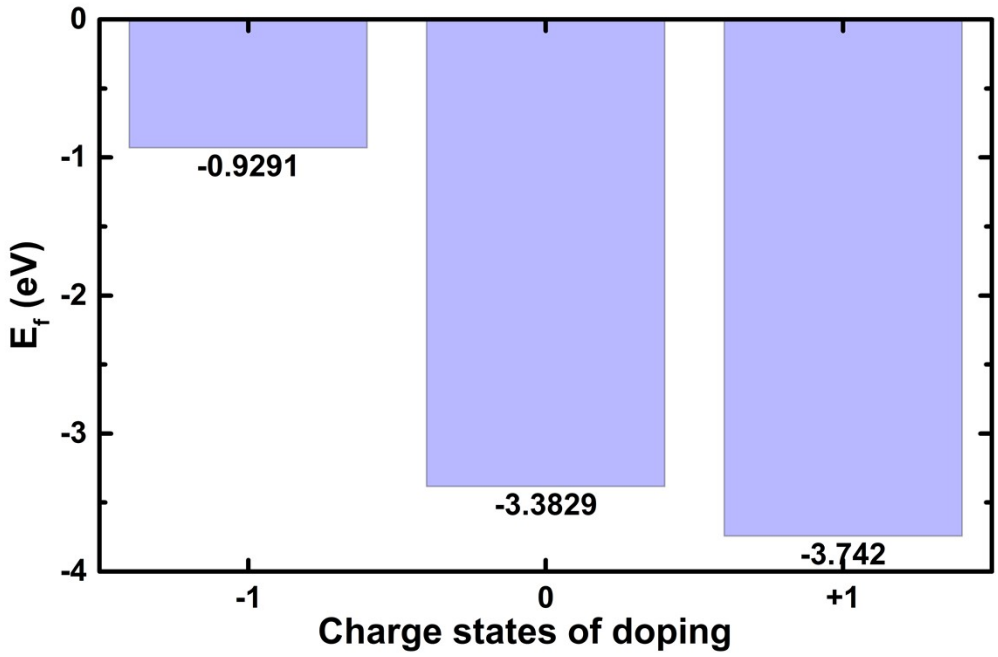

Figure S2: Fermi level of 1Fe@PbI_2 system at different charge states of impurity.

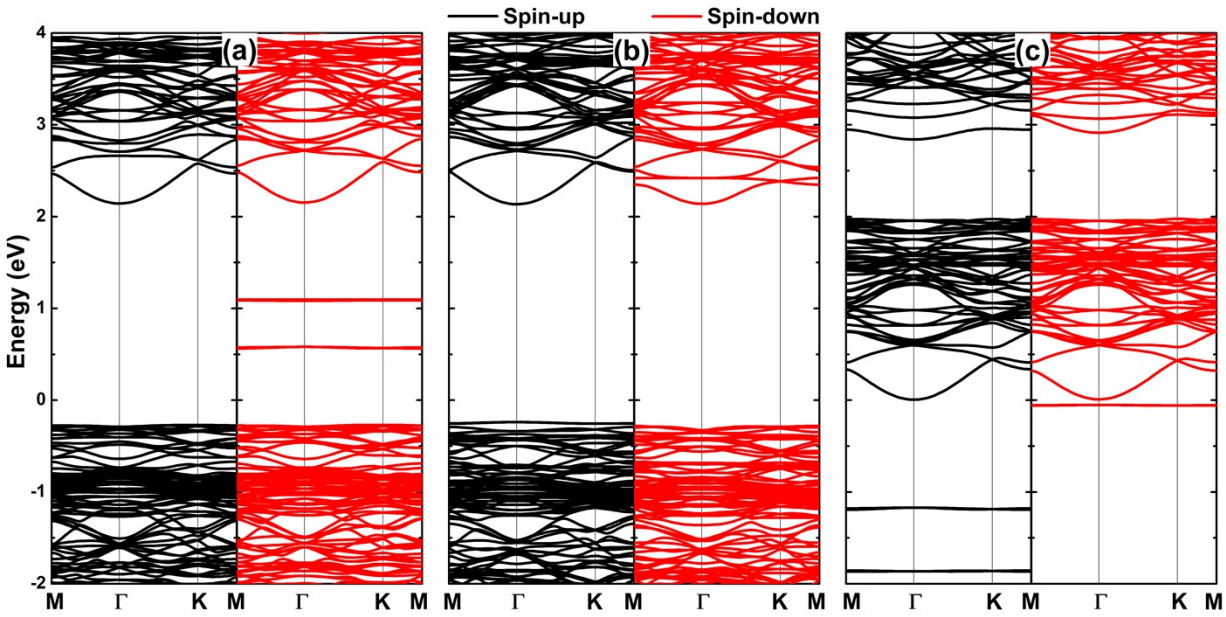

Figure S3: Spin-resolved band structure of 1Fe@PbI_2 monolayer at different charge states of impurity: (a) +1 state, (b) Neutral state, and (c) -1 state (The Fermi level is set to 0 eV in all cases).