Electronic Supplementary Material (ESI) for RSC Advances.

Tuning MoSO monolayer prop erties for opto electronic and spintronic applications: Effect of external strain, vacancy, and doping

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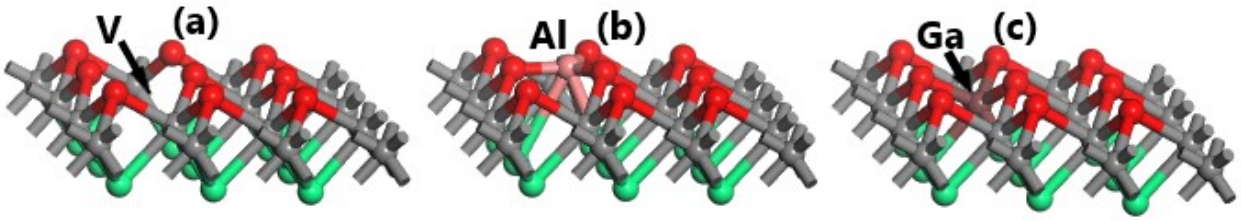

Figure S1: Optimized atomic structure of (a) Mo_V, (b) Mo_{Al}, and (c) Mo_{Ga} system.

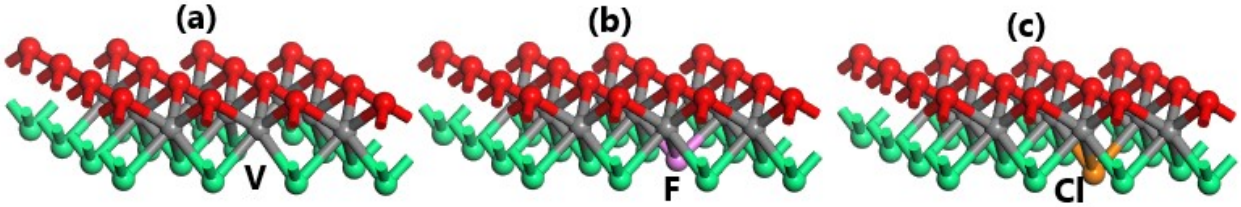

Figure S2: Optimized atomic structure of (a) S_V, (b) S_F, and (c) S_{Cl} system.

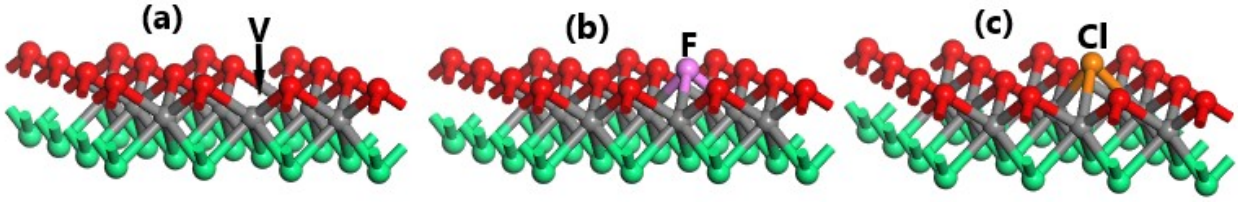

Figure S3: Optimized atomic structure of (a) O_V, (b) O_F, and (c) O_{Cl} system.

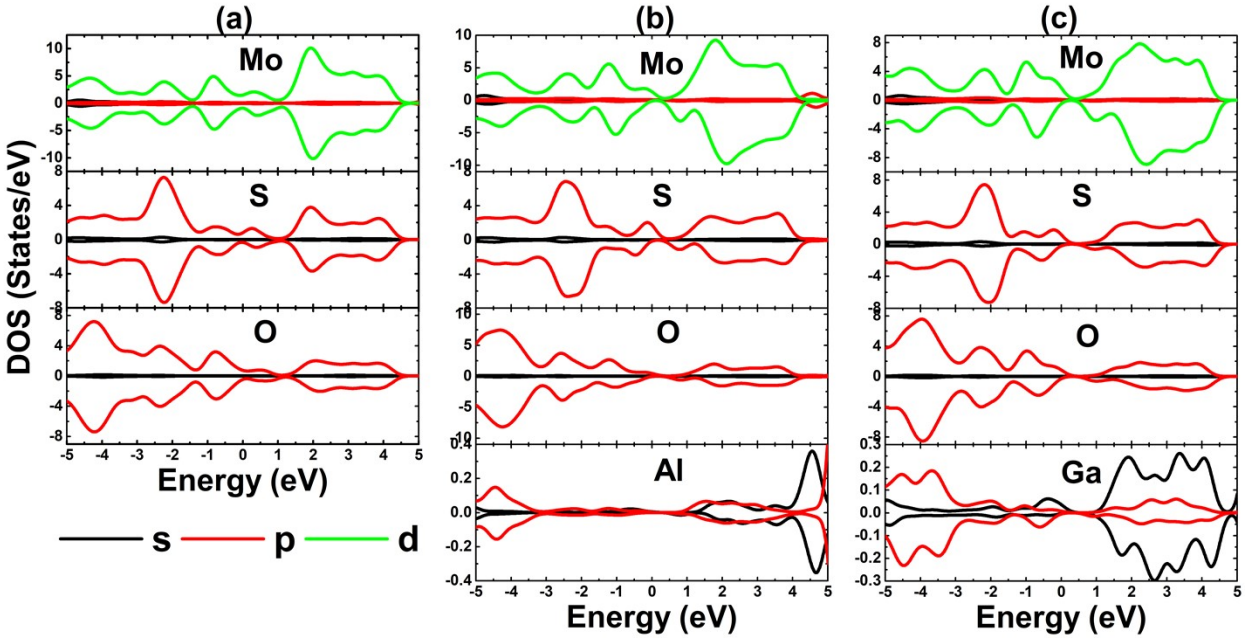

Figure S4: Partial density of states of (a) Mo_V, (b) Mo_{Al}, and (d) Mo_{Ga} system.

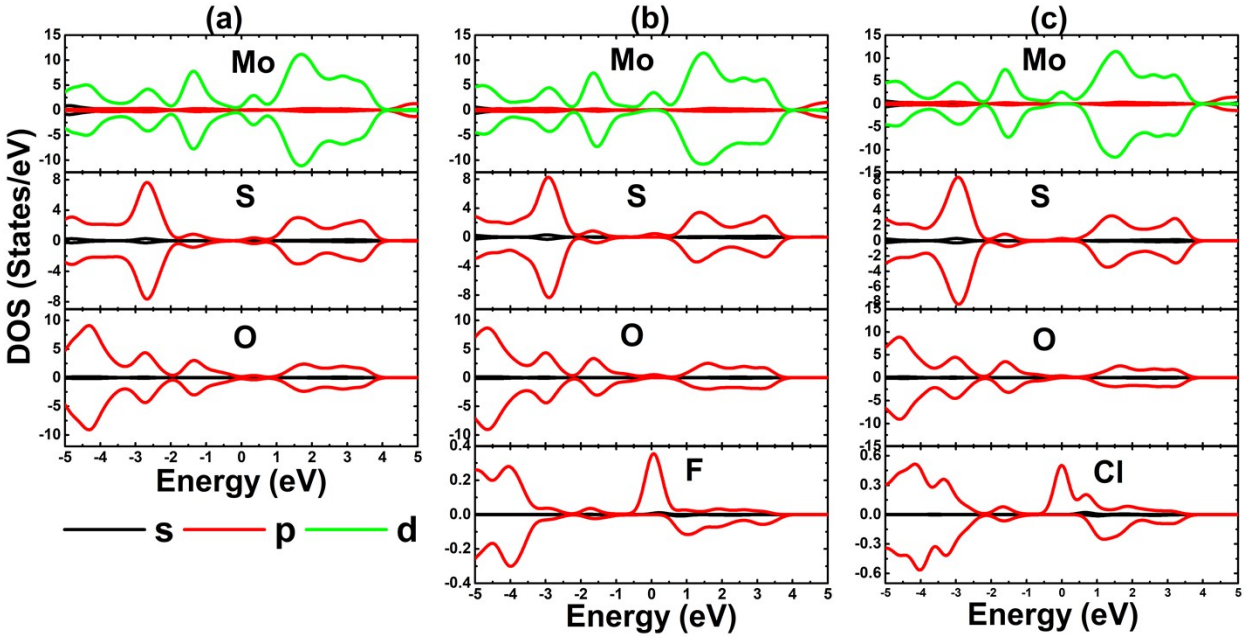

Figure S5: Partial density of states of (a) S_V, (b) S_F, and (d) S_{Cl} system.

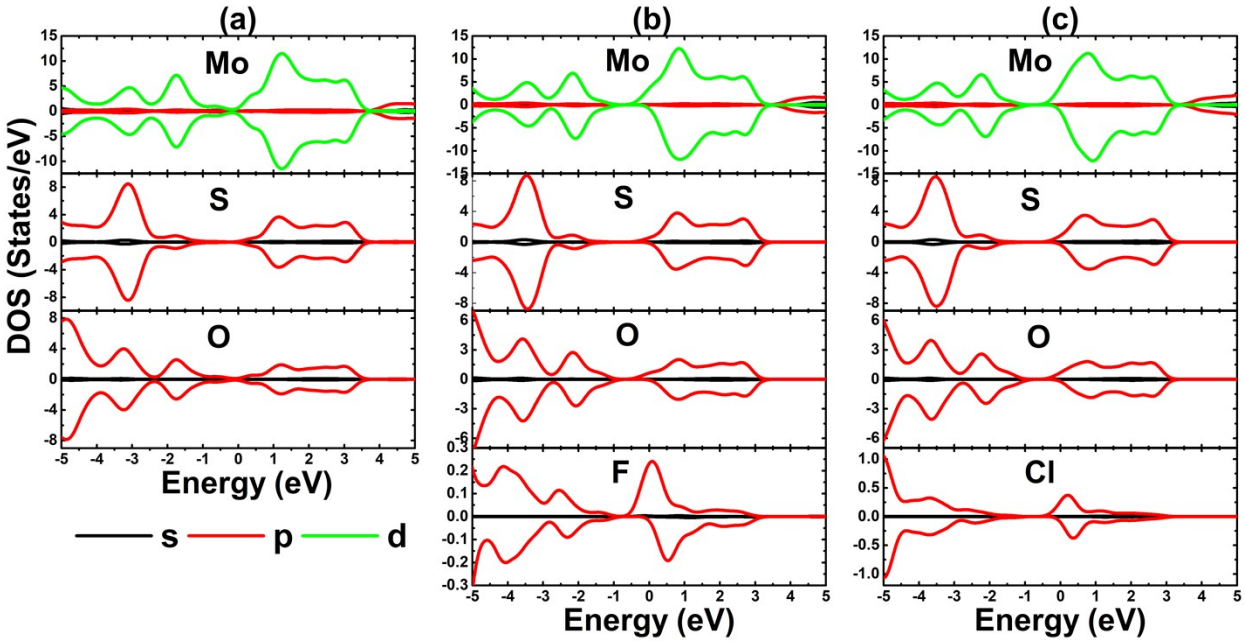

Figure S6: Partial density of states of (a) O_V, (b) O_F, and (d) O_{Cl} system.