

Supplementary Information

Au clusters adsorption on the perfect and the defective MoS₂ monolayers: structural and electronic properties

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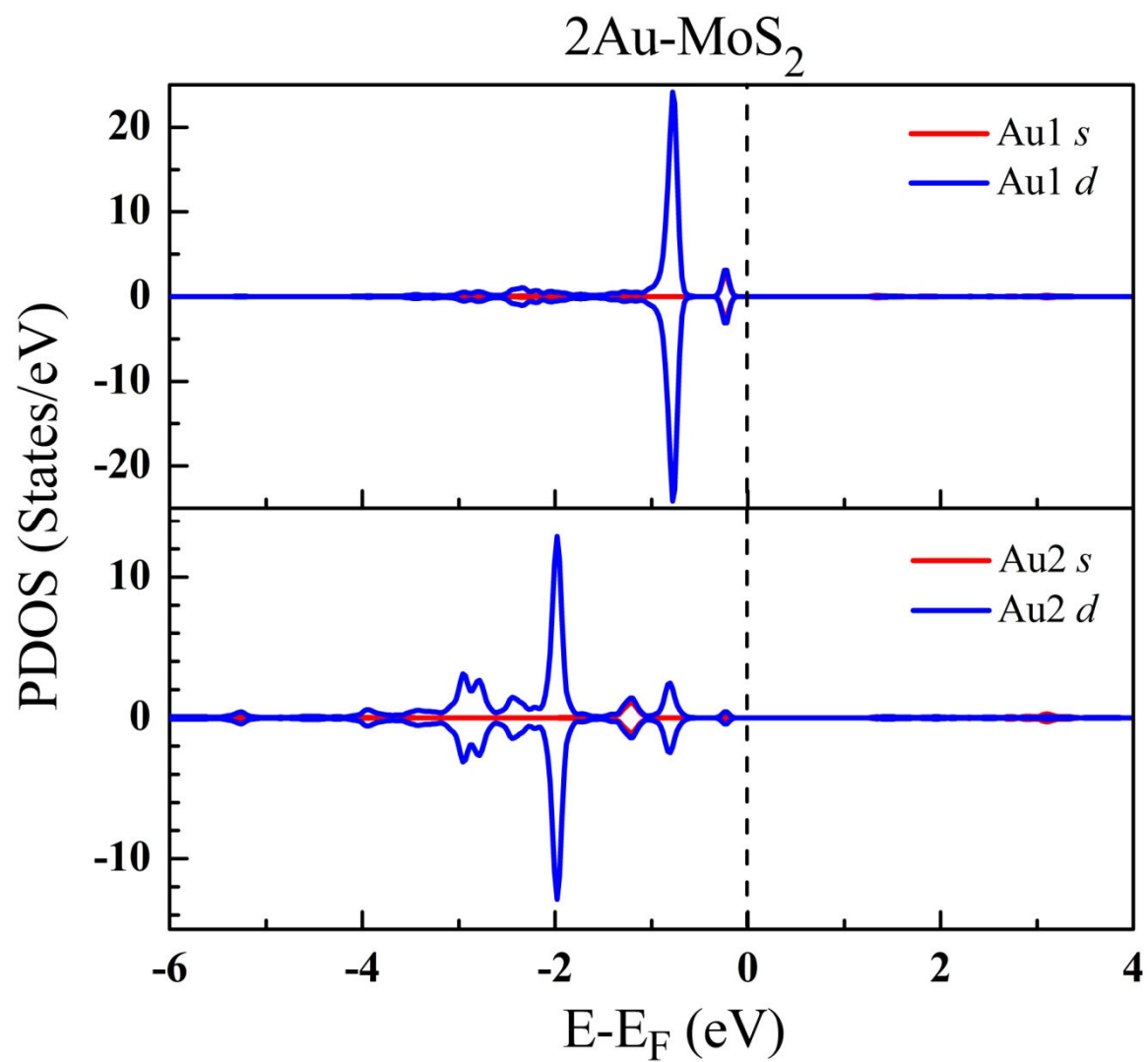


Fig. S1 The PDOSs of all Au atoms in 2Au-MoS_2 system.

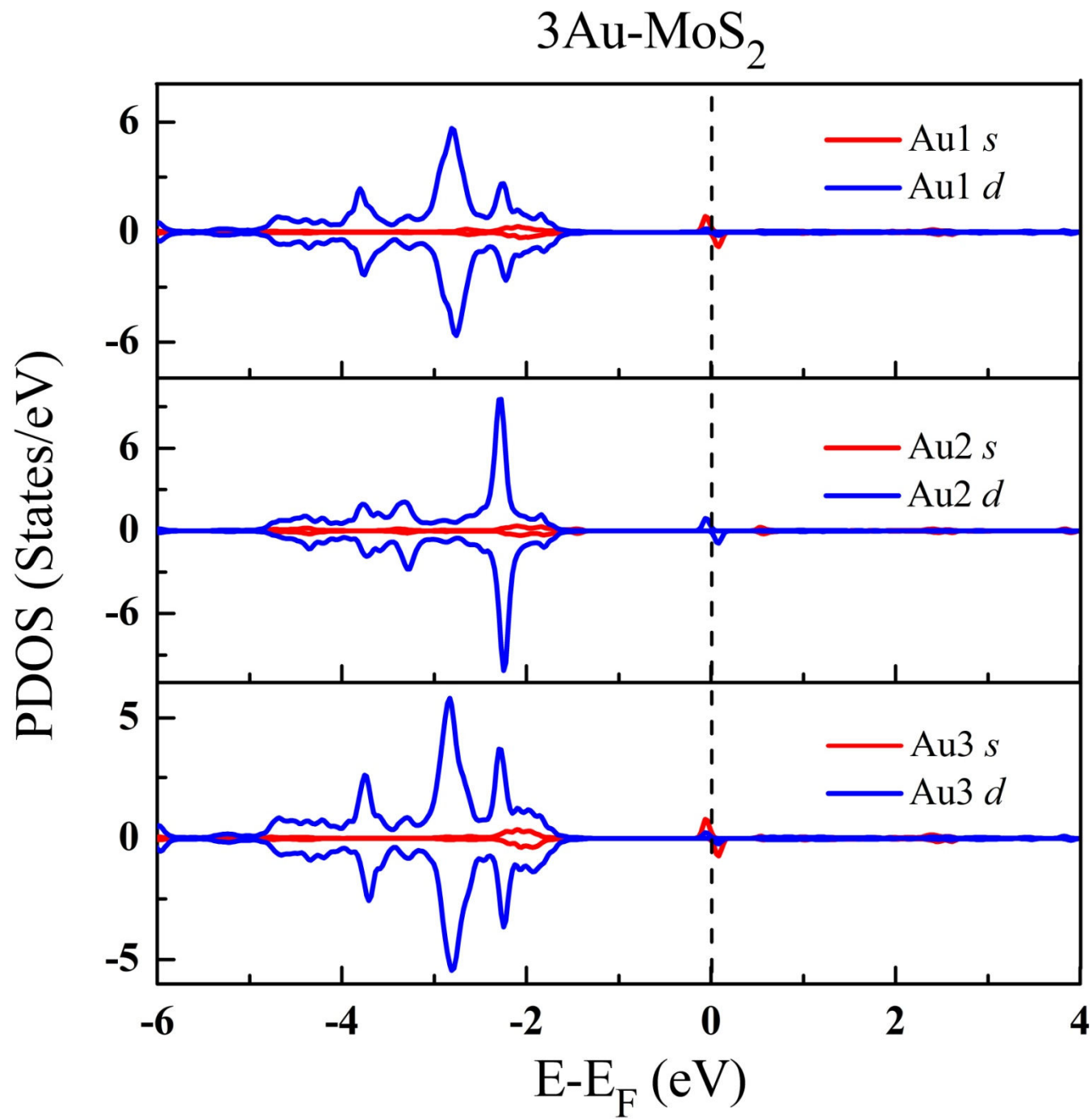


Fig. S2 The PDOSs of all Au atoms in 3Au-MoS_2 system.

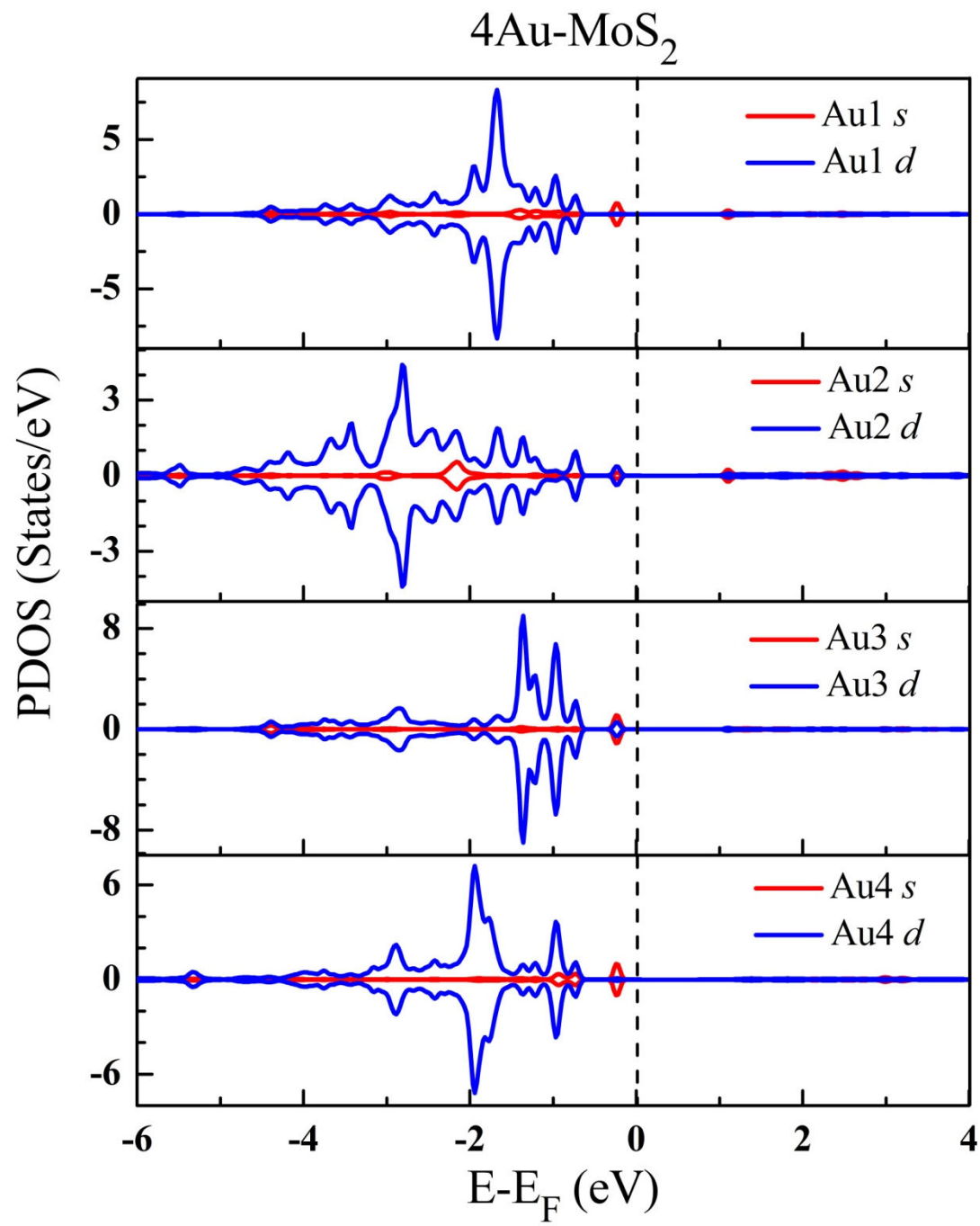


Fig. S3 The PDOSs of all Au atoms in 4Au-MoS_2 system.

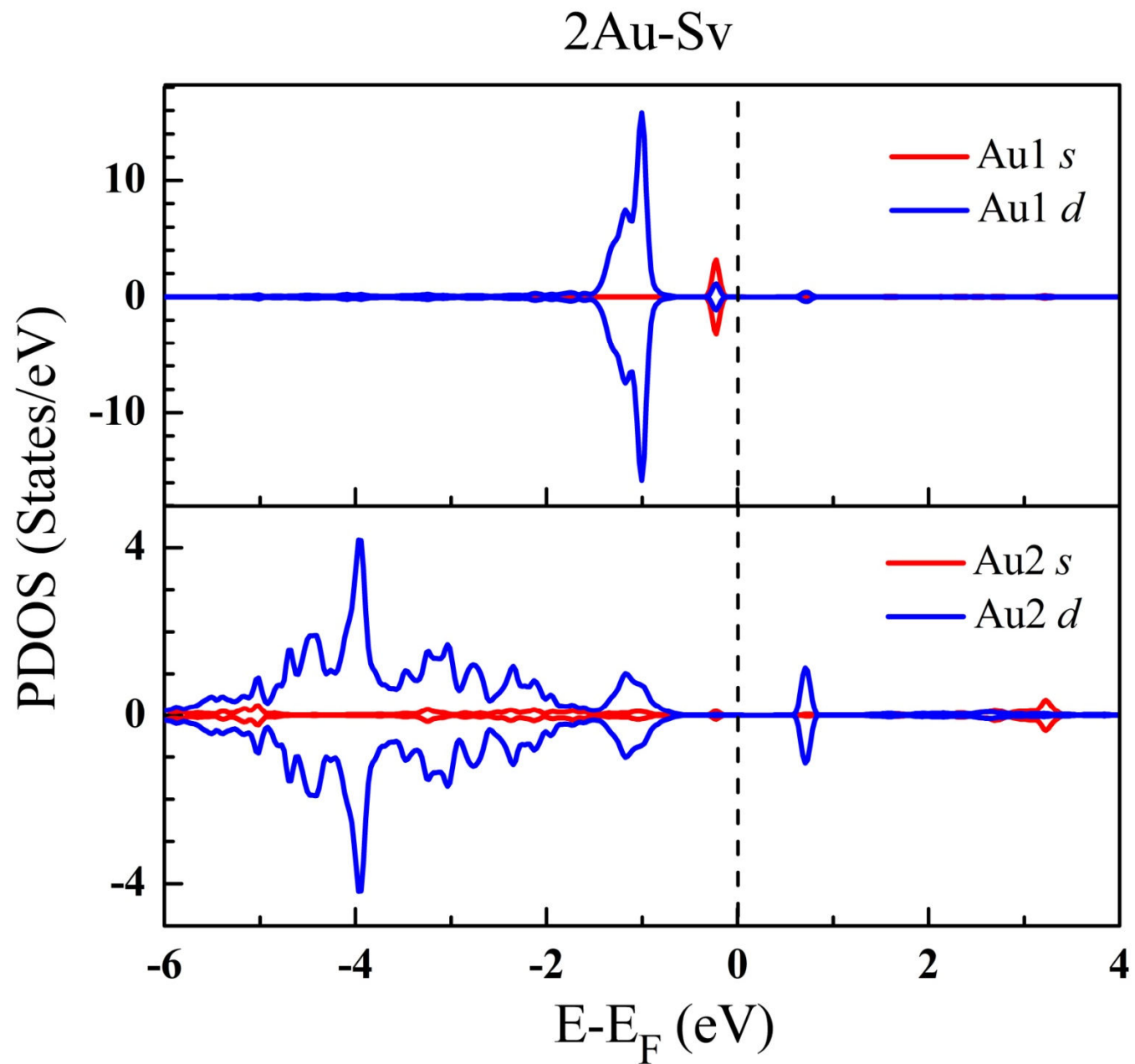


Fig. S4 The PDOSs of all Au atoms in 2Au-Sv system.

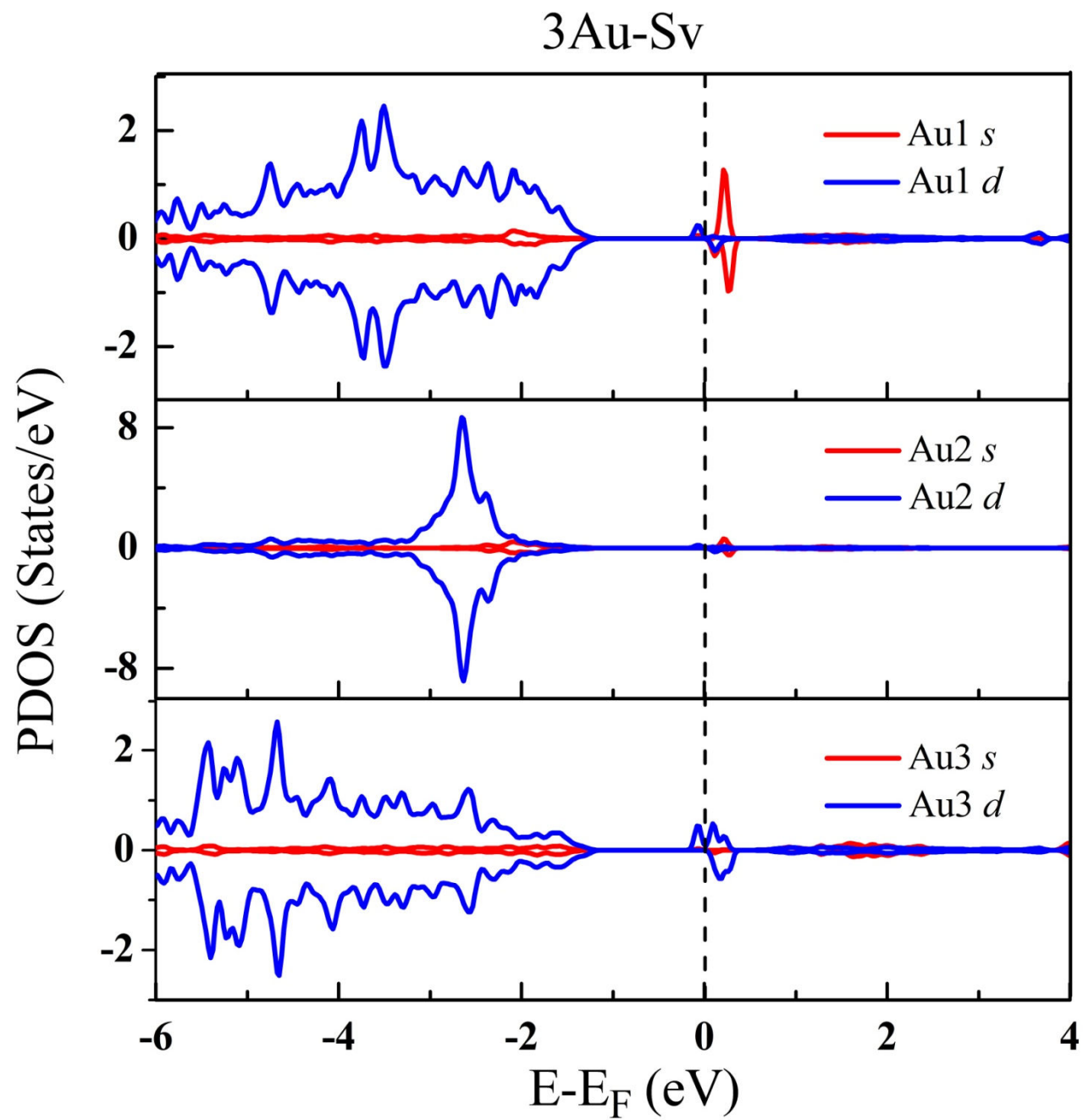


Fig. S5 The PDOSs of all Au atoms in 3Au-Sv system.

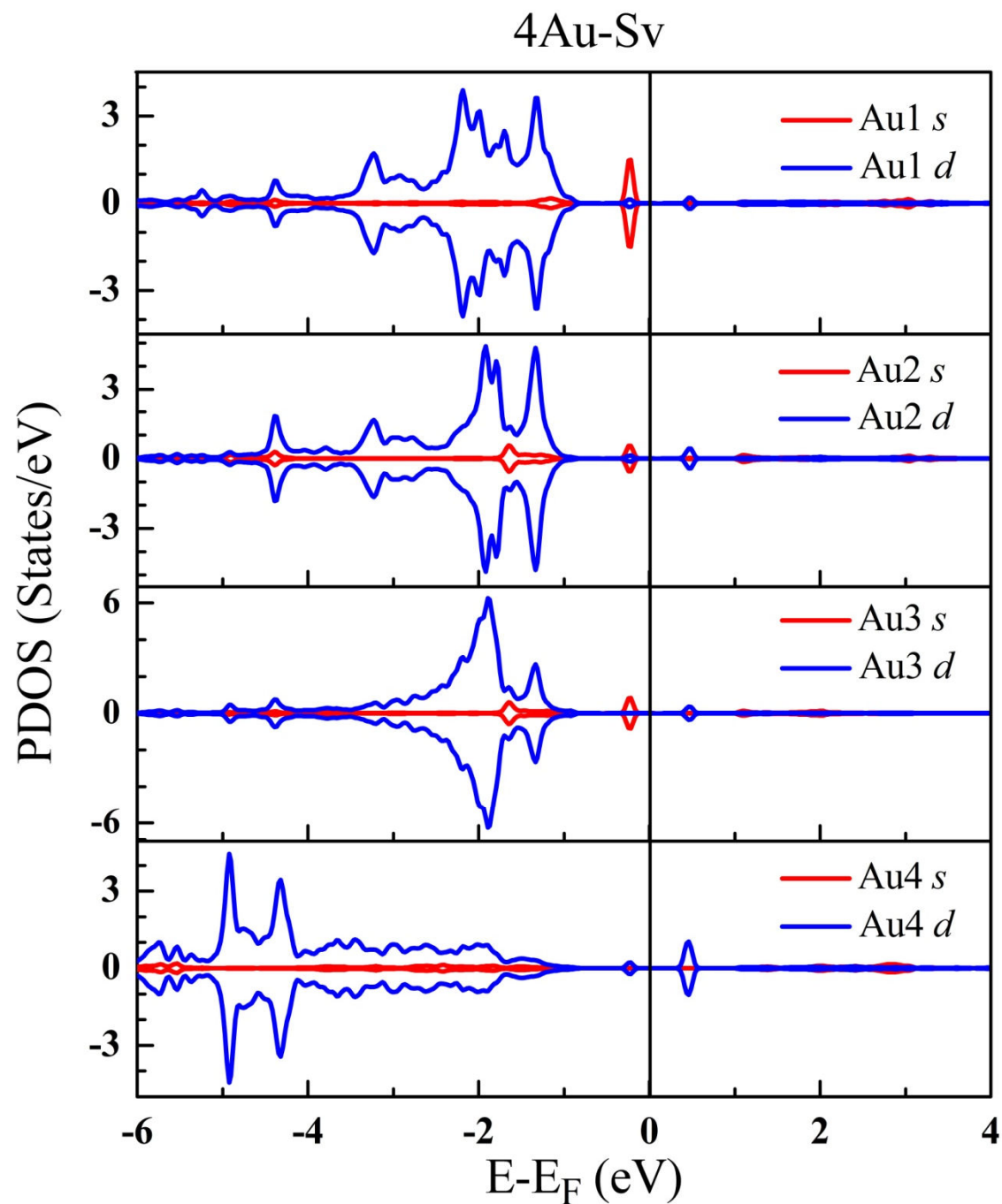


Fig. S6 The PDOSs of all Au atoms in 4Au-Sv system.

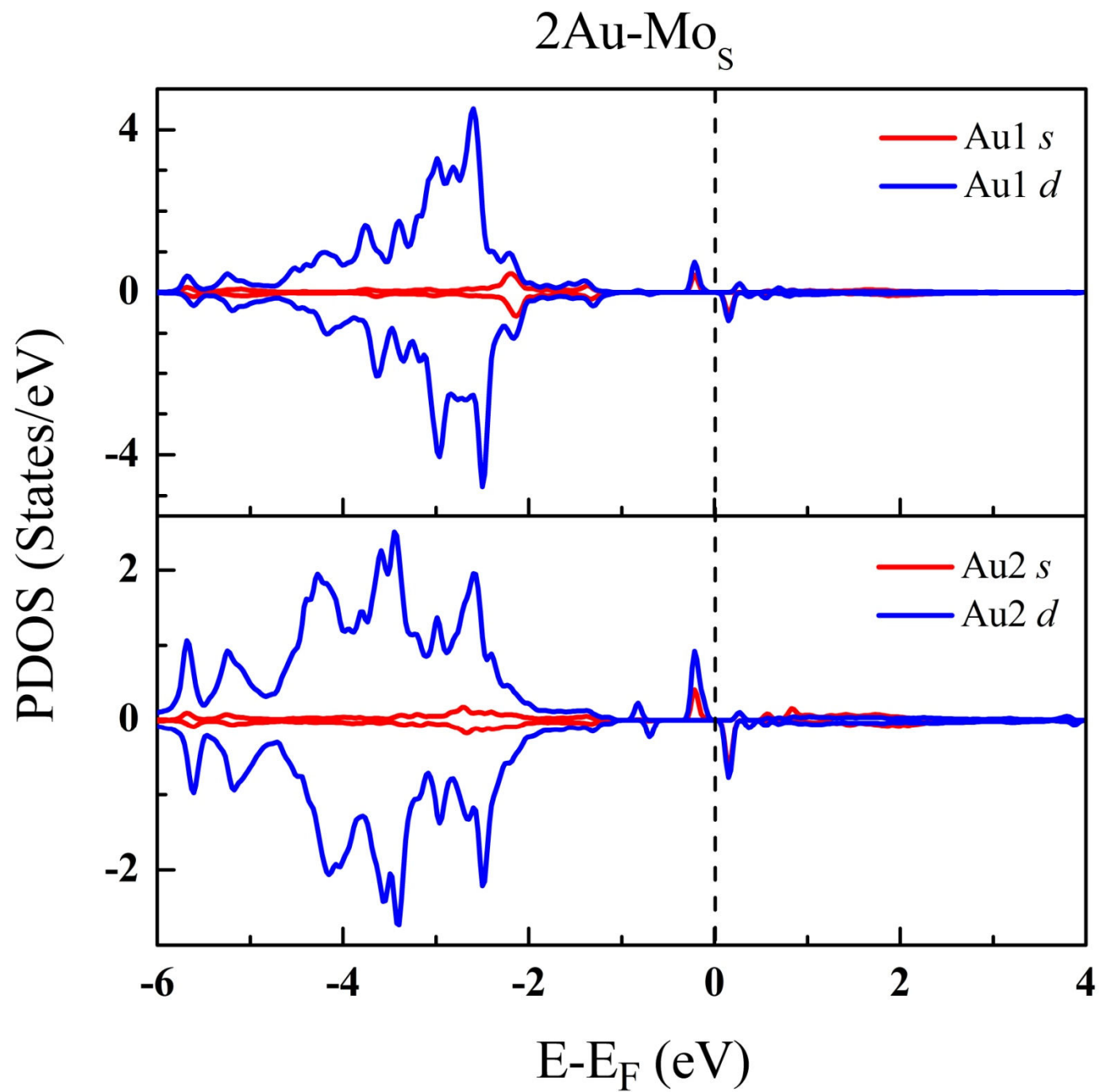


Fig. S7 The PDOSs of all Au atoms in 2Au-Mo_s system.

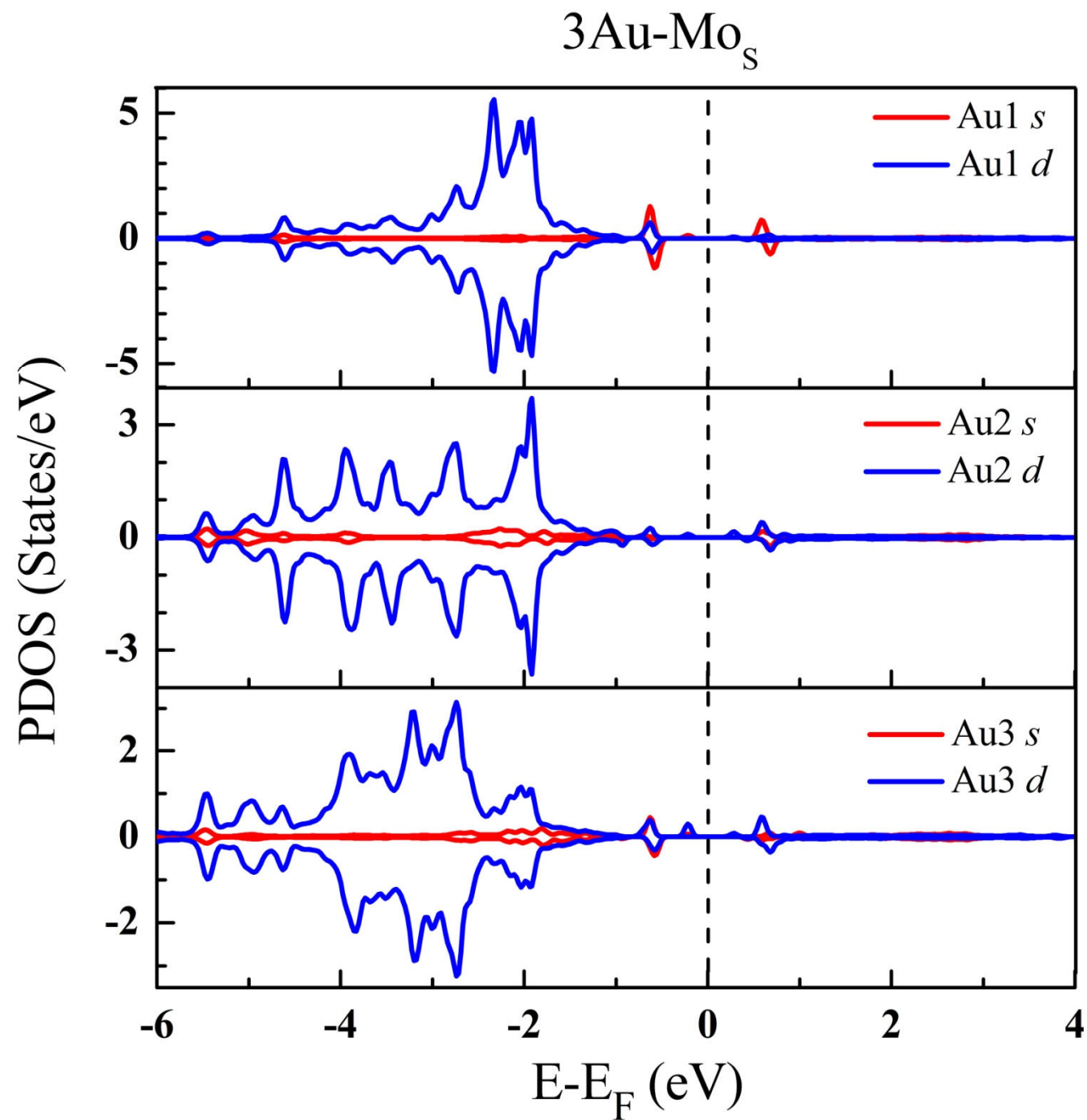


Fig. S8 The PDOSs of all Au atoms in 3Au-Mo_s system.

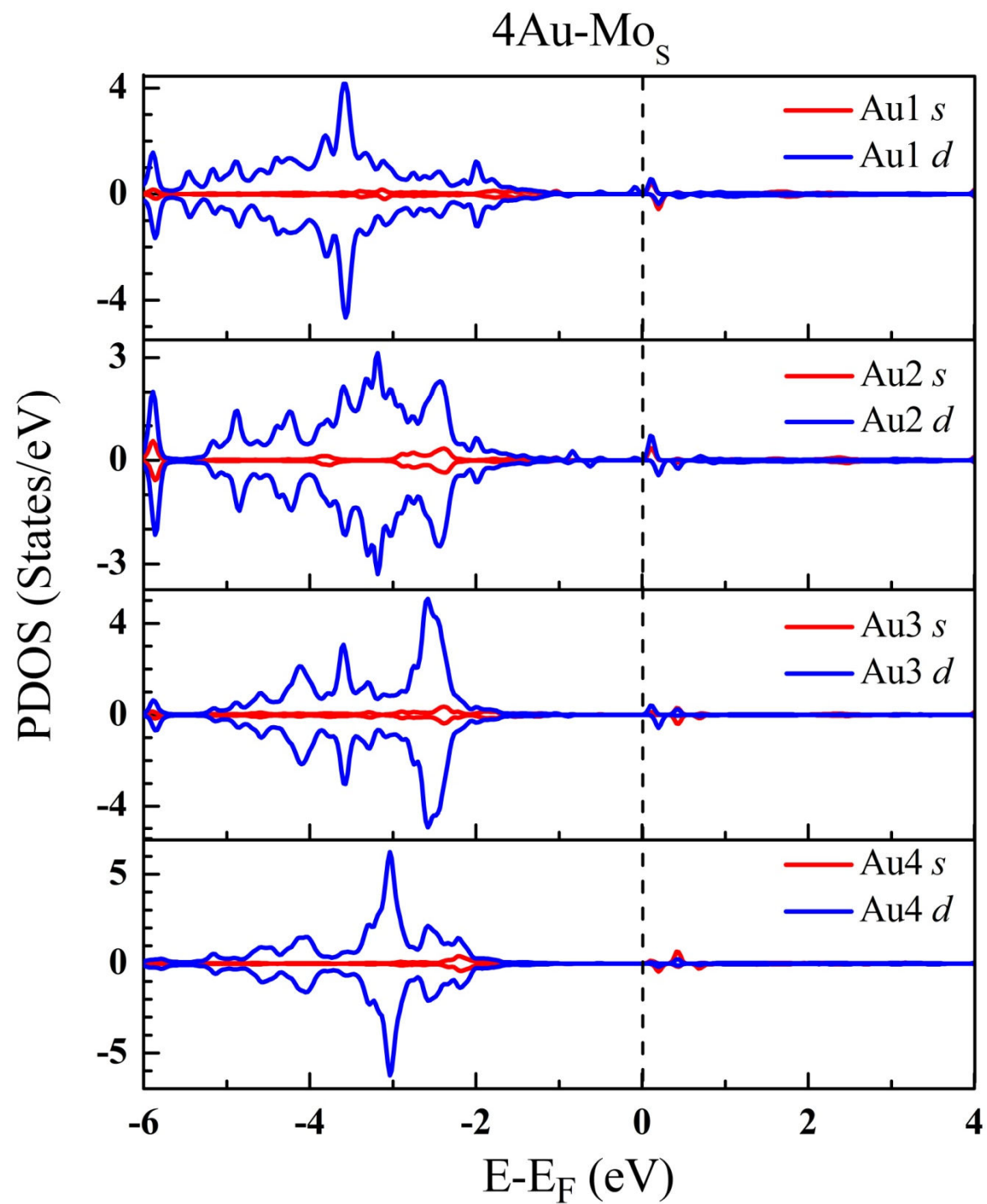


Fig. S9 The PDOSs of all Au atoms in 4Au-Mo_s system.