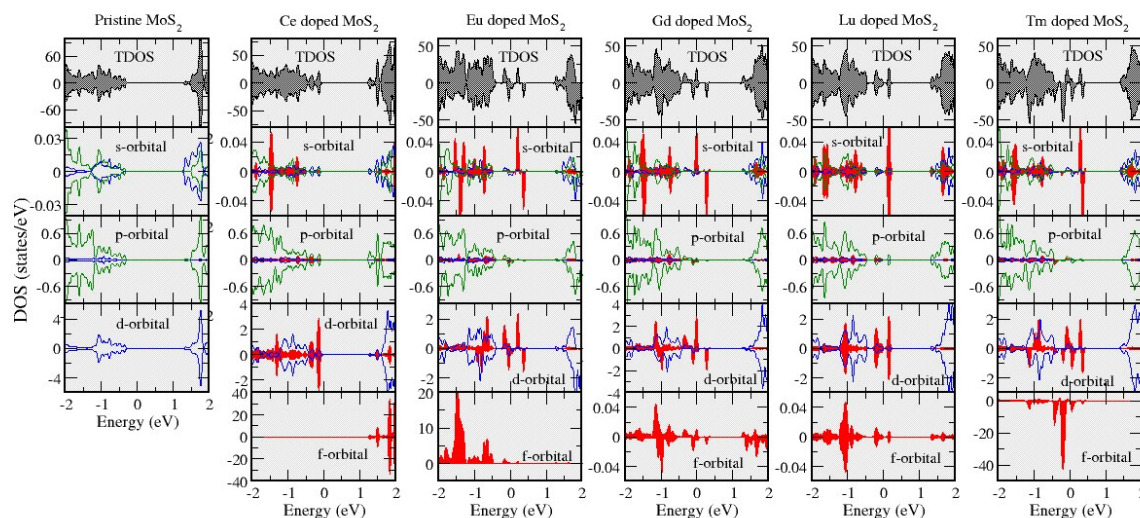


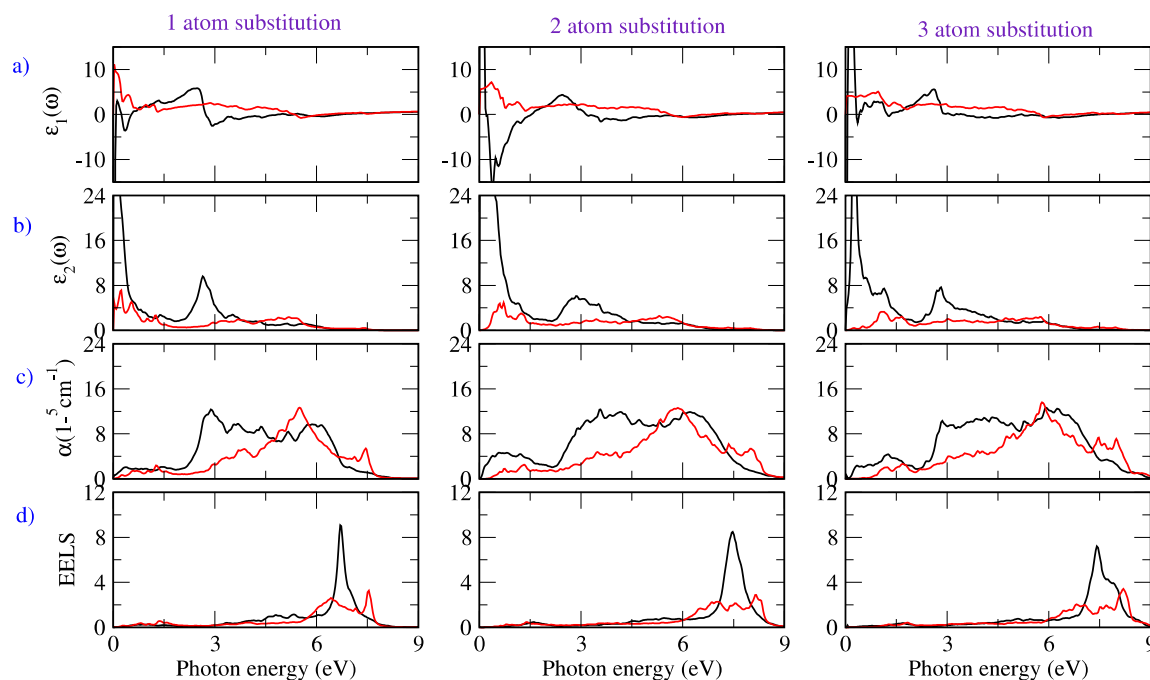
Supplementary material

Controlling the magnetic and optical response of MoS₂ monolayer by lanthanide substitutional doping: a first-principles study

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S 1: Calculated PDOS for pristine and doped systems. The Blue, Green and Red lines represents the Mo, S and dopant orbitals respectively



S 2: Calculated optical properties of Tm doped MoS₂ monolayer at 1, 2 and 3 atom substitutional doping for E-field polarization parallel to the xy-plane (black line), and

perpendicular to the xy-plane (red line). Panels a), b), c) and d) presents the spectra for real part of the dielectric function, imaginary part of the dielectric function, absorption co-efficient, and the EELS respectively.