

Electronic Supplementary Information

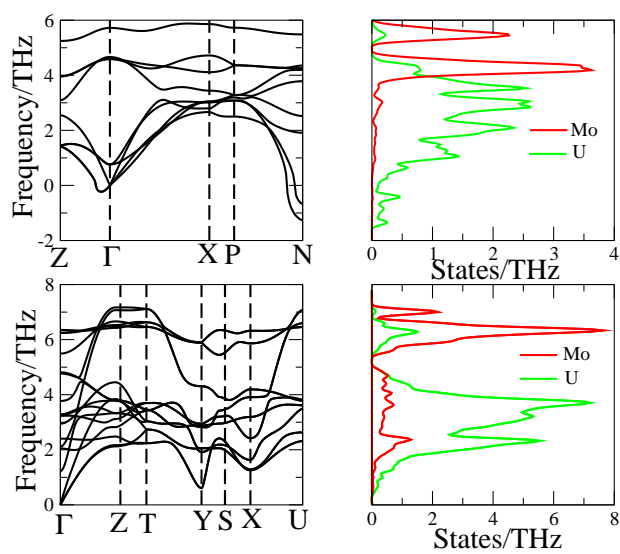


Fig.S1 (color online) The calculated phonon spectra and DOS of the  $I4/mmm$  (upper panels) and the  $Pmmn$  phases (lower panels) within DFT+D