Evaluating Sulfur as a P-type Dopant in Cu_3N Using Ab initio Methods

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Supplementary Material

Figure S1. PDOS of Cu_3N:S alloy with a -2 charge + Hubbard

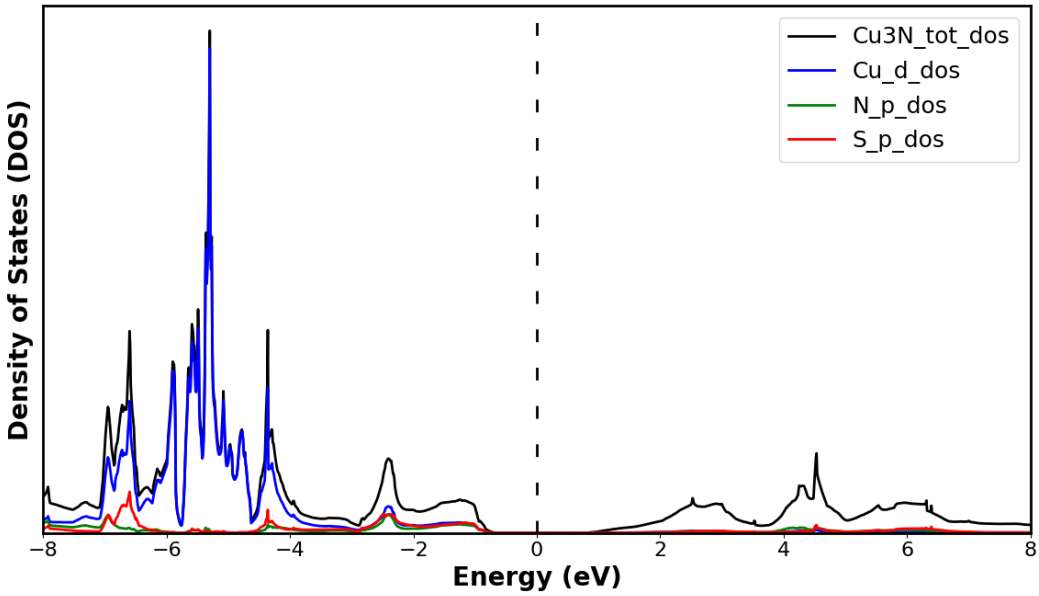

Figure S2. Absorption coefficient of Cu_3N: Hubbard calculation

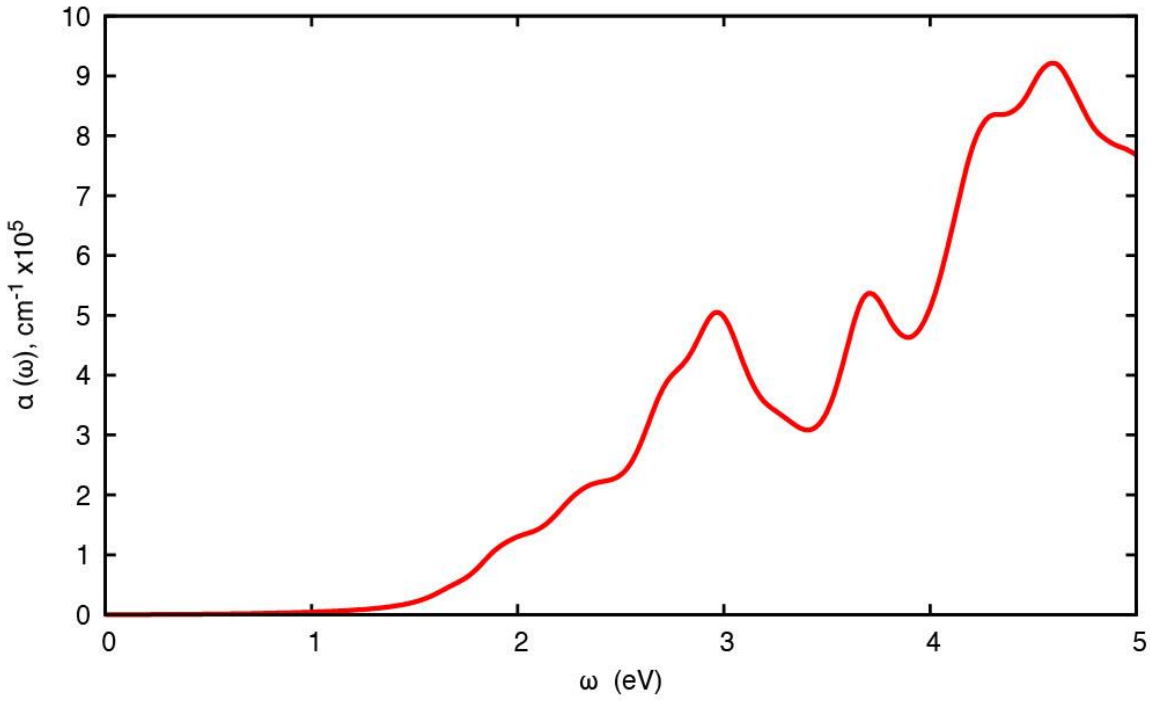

Figure S3. Band structure of intrinsic Cu_3N in the supercell configuration using Hubbard.

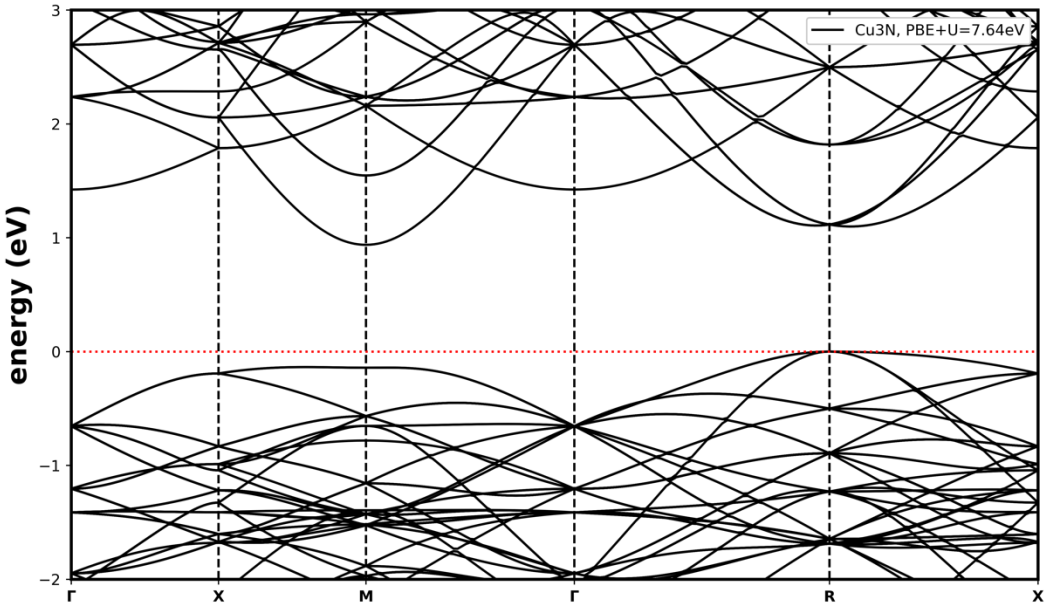

Figure S4. Band structure of sulfur-doped Cu_3N in the supercell configuration using Hubbard.