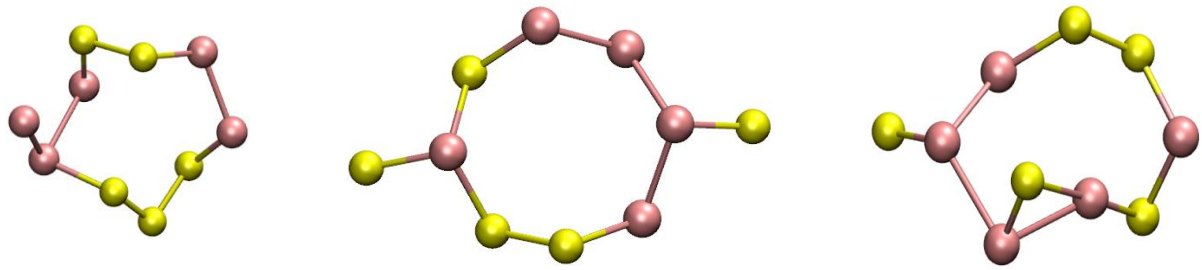
Electronic Supplementary Material (ESI) for Nanoscale Advances.



0.593eV (a) 0.885eV (b) 1.266eV (c)

Fig. S1. High energy isomers of Se_5Te_5 clusters

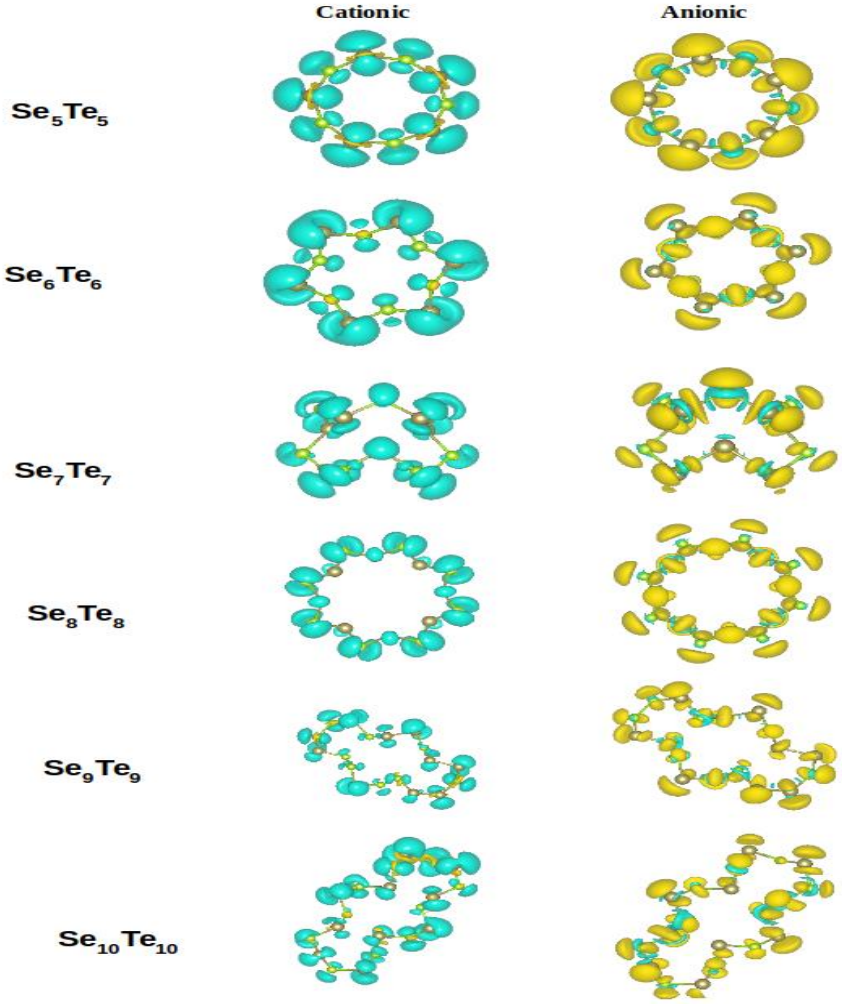


Fig. S2. Charge density difference profile of cationic and anionic Se_nTe_n clusters.

Charge density difference is determined from the expression, $\delta\rho(r) = \rho(r)^{-/+} - \rho(r)^{0}$, here $\rho(r)^{-/+}$ and $\rho(r)^{0}$ represent the charge density of the charged and neutral cluster, respectively. In charge density profile yellow colour represent accumulation of charge, electron charge, and cyan colour represent the depletion of charge, hole charge. Charge density difference profile of charged system reveals that the electron and hole charge does not spill over to vacuum region but is localized on the cluster.

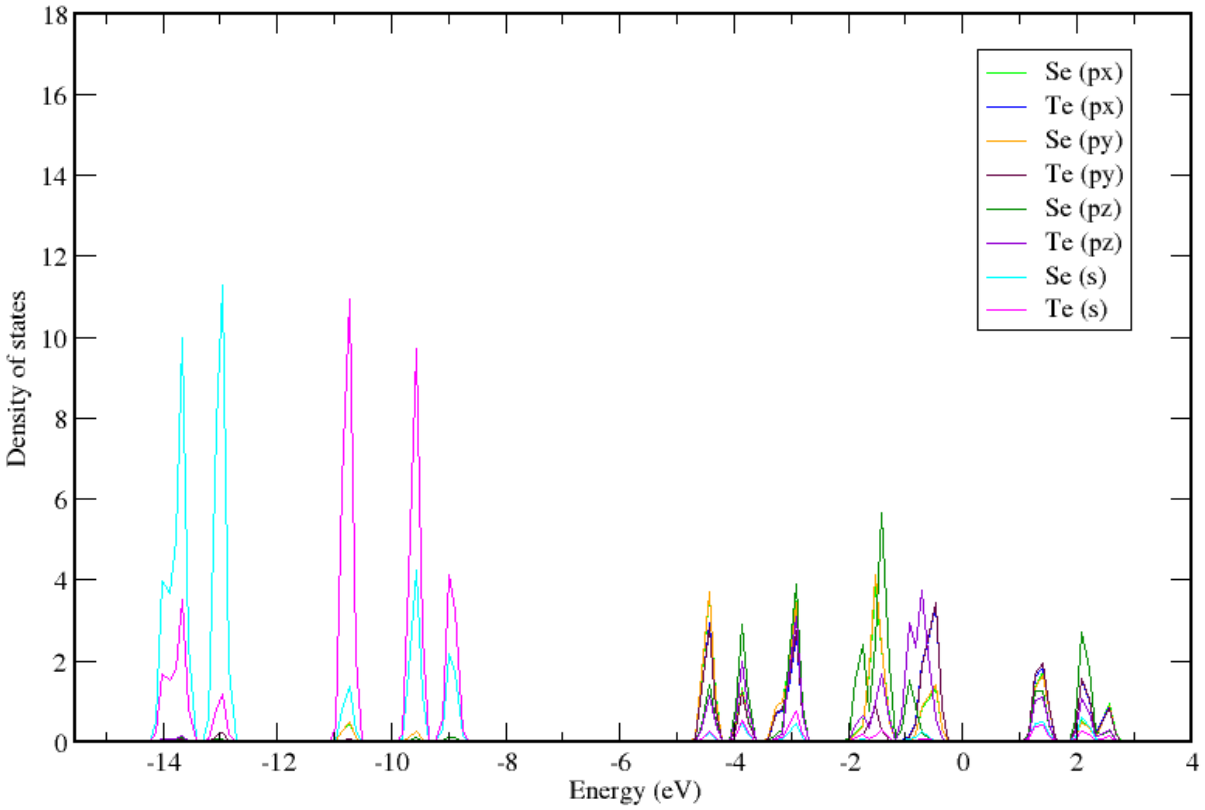


Fig. S3. Angular momentum and site projected density of states, for n=5. Fermi energy is shifted to 0 eV.

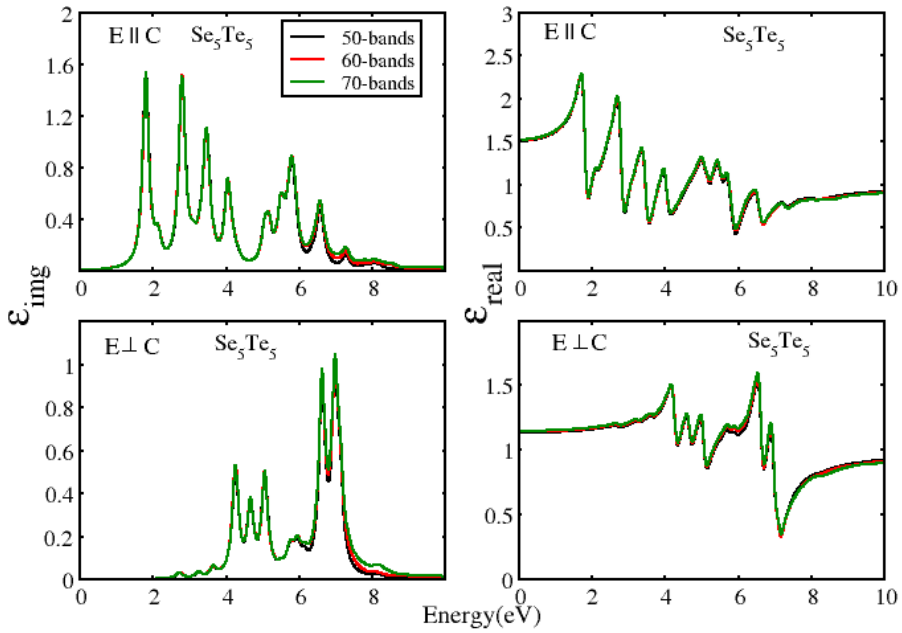


Fig. S4. Dielectric function with varying number of empty states for Se_5Te_5

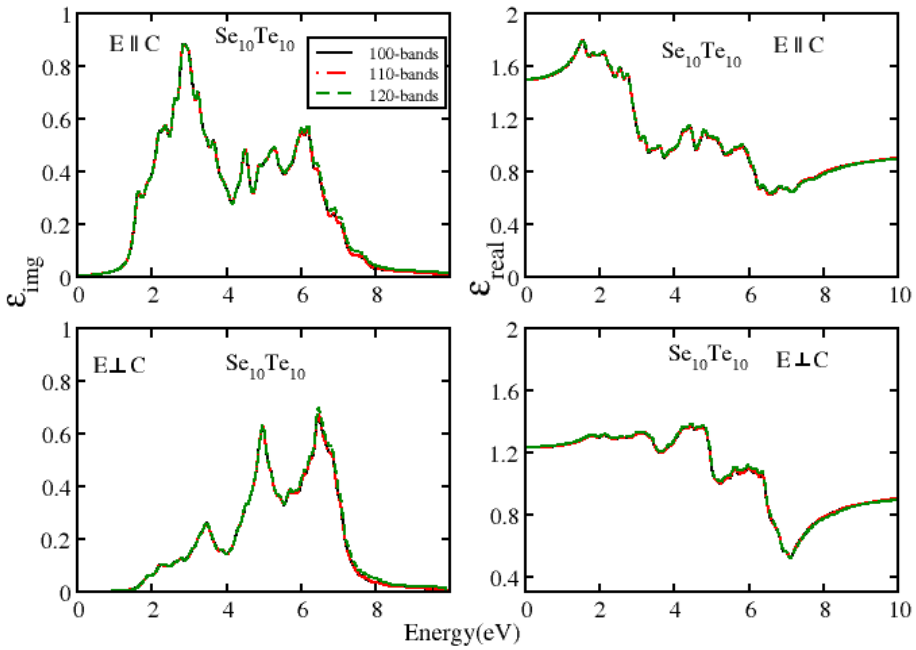


Fig. S5. Dielectric function with varying number of empty states for $Se_{10}Te_{10}$

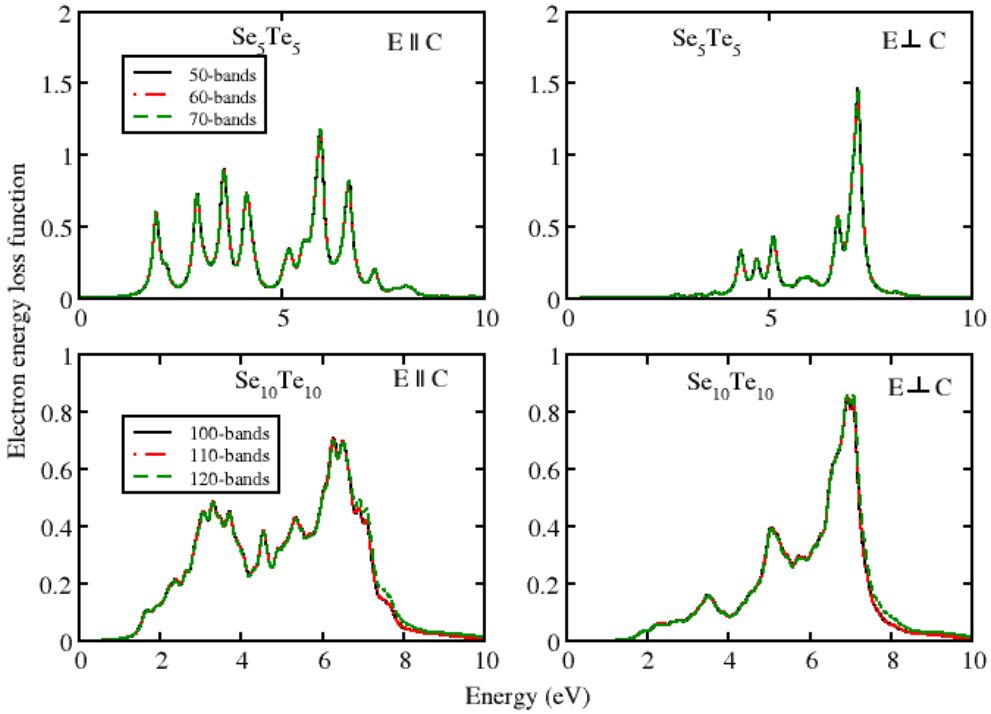


Fig. S6. Electron energy loss function with varying number of empty states