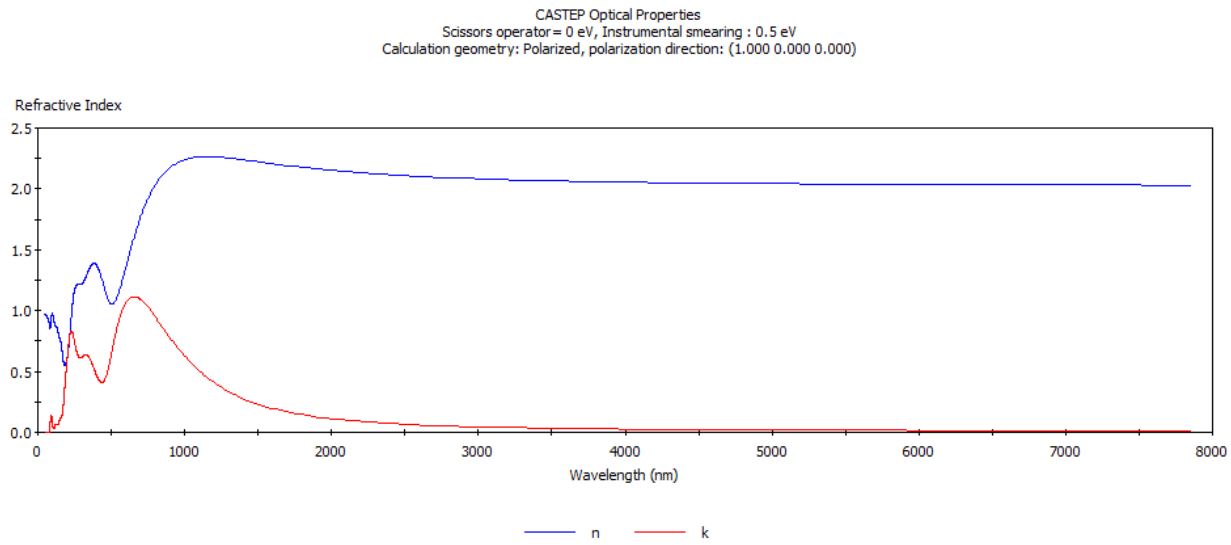
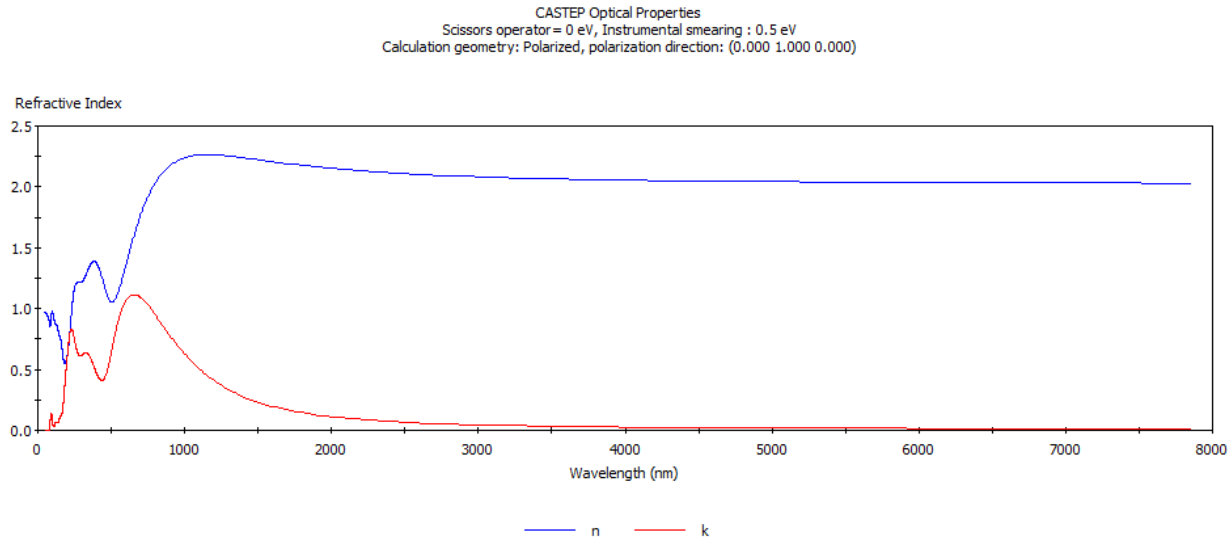
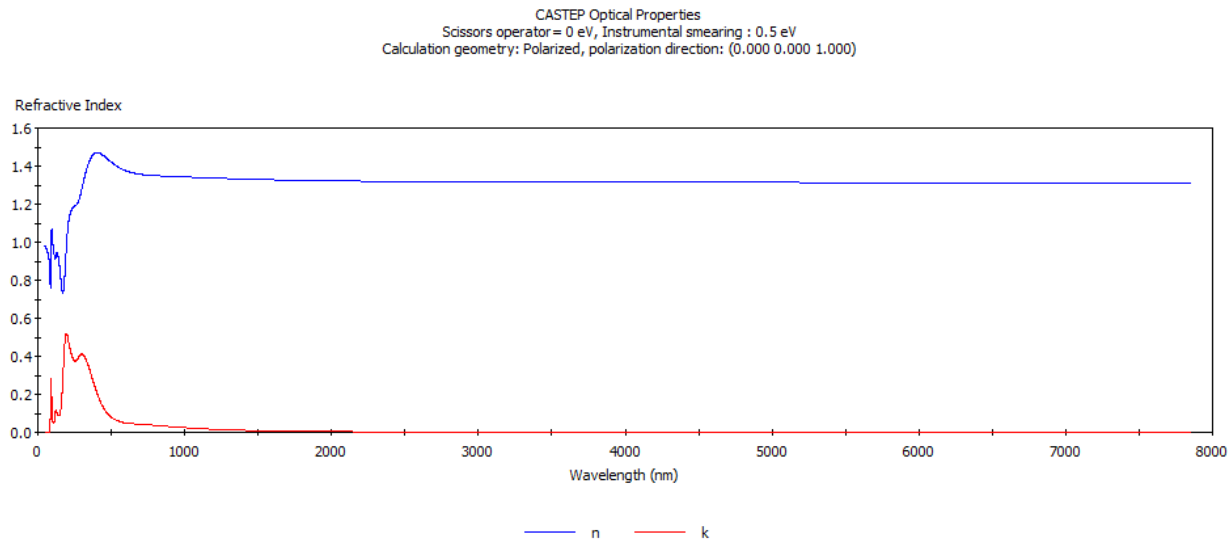
Electronic Supplementary Material (ESI) for CrystEngComm.



S 1. real and imaginary part of Refractive index along 010 direction



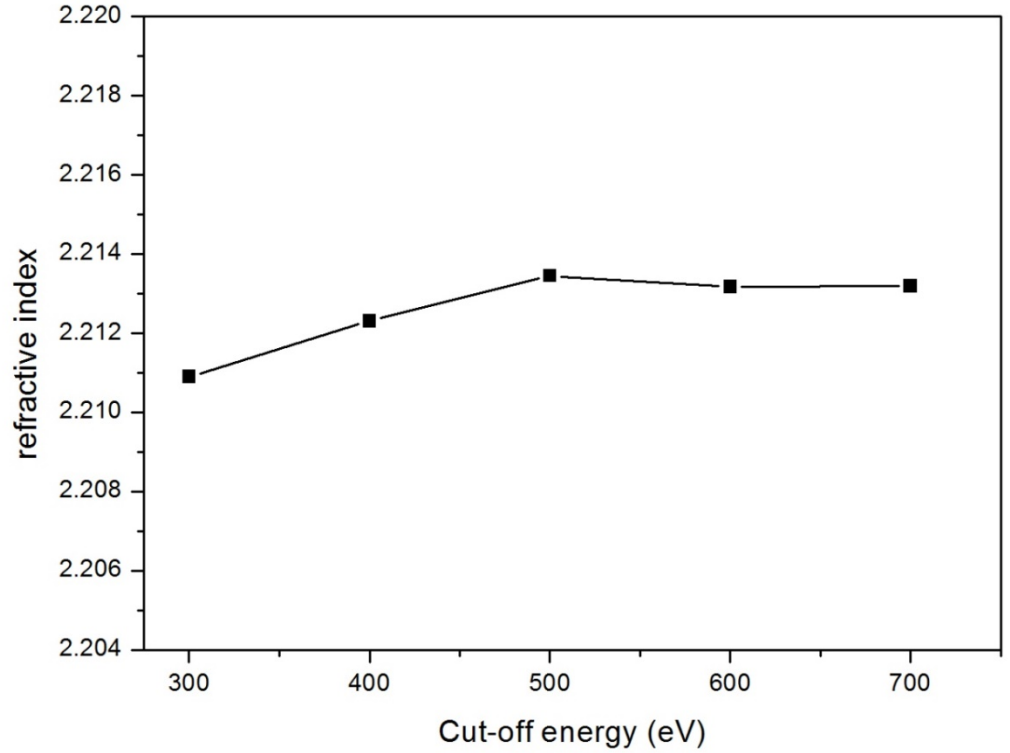
S 2. real and imaginary part of Refractive index along 010 direction



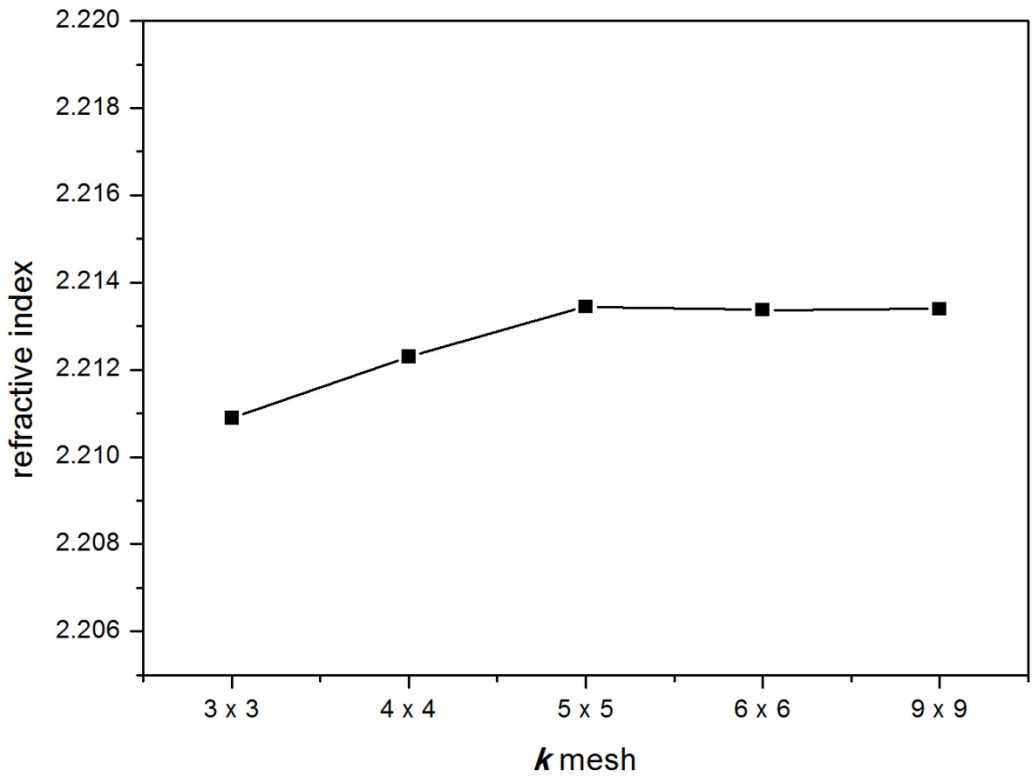
S 3. real and imaginary part of Refractive index along 001 direction

Convergence test

The accuracy of refractive index (n_1) at 1550 nm is calculated for five different plane wave cut-off energies. The chosen values of refractive index at 400 eV and ***k*** point mesh (4×4) were found to converge within 0.00086 with respect to higher values of refractive index at 700 eV and 9x 9x1 k point mesh.



S 4 Convergence test on the dependence of refractive index on cut-off energy



S 5 Convergence test on the dependence of refractive index on ***k*** point mesh.