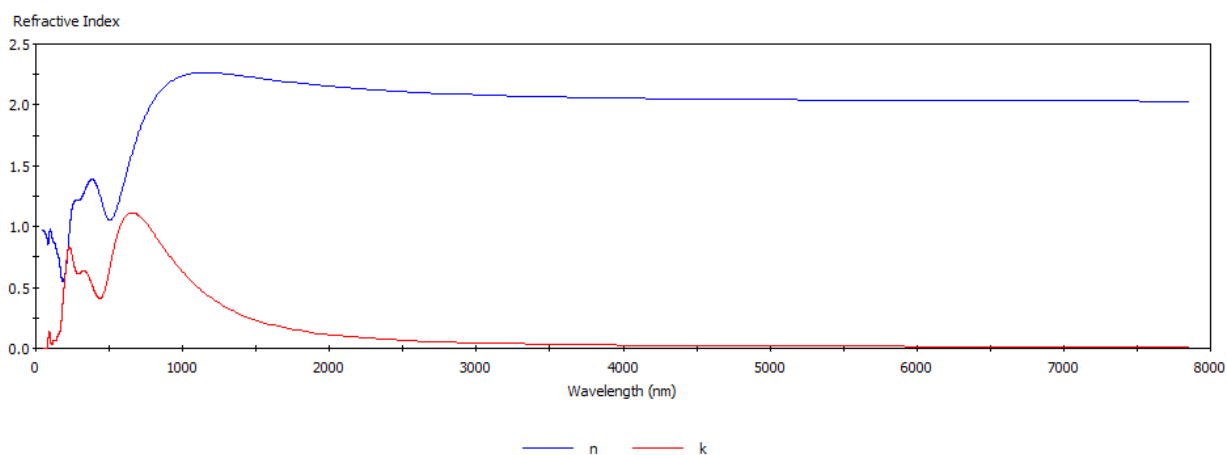
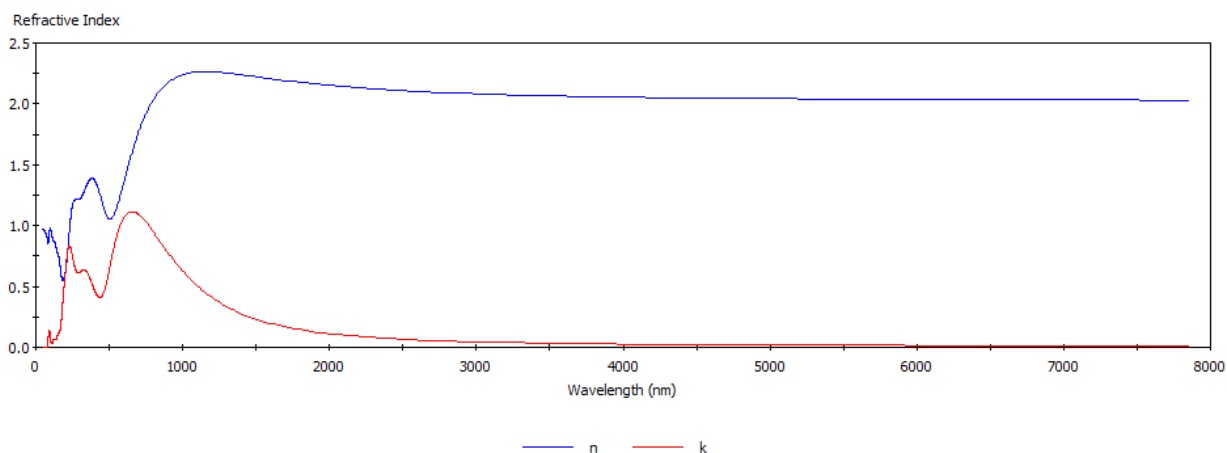


CASTEP Optical Properties
Scissors operator = 0 eV, Instrumental smearing : 0.5 eV
Calculation geometry: Polarized, polarization direction: (1.000 0.000 0.000)



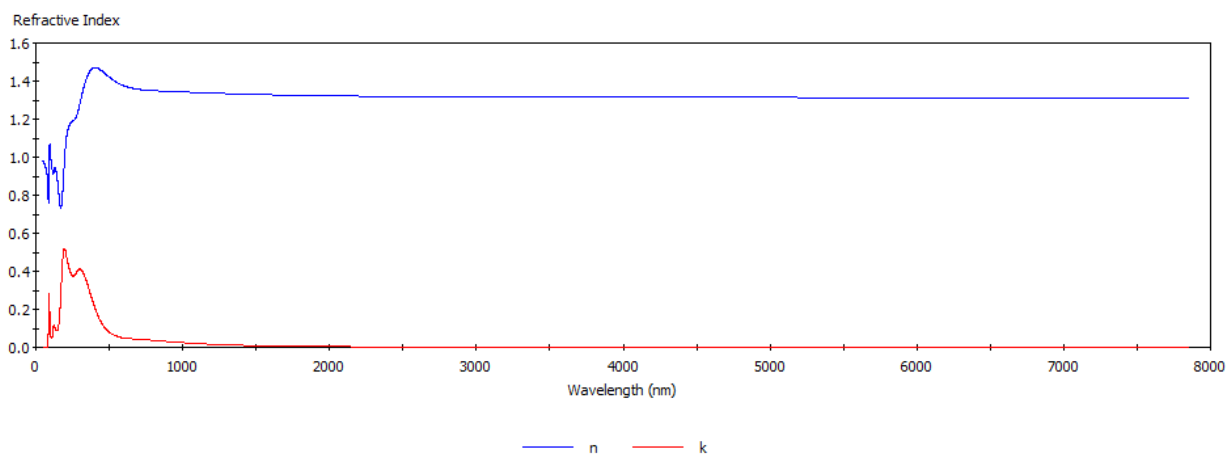
S 1. real and imaginary part of Refractive index along 010 direction

CASTEP Optical Properties
Scissors operator = 0 eV, Instrumental smearing : 0.5 eV
Calculation geometry: Polarized, polarization direction: (0.000 1.000 0.000)



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

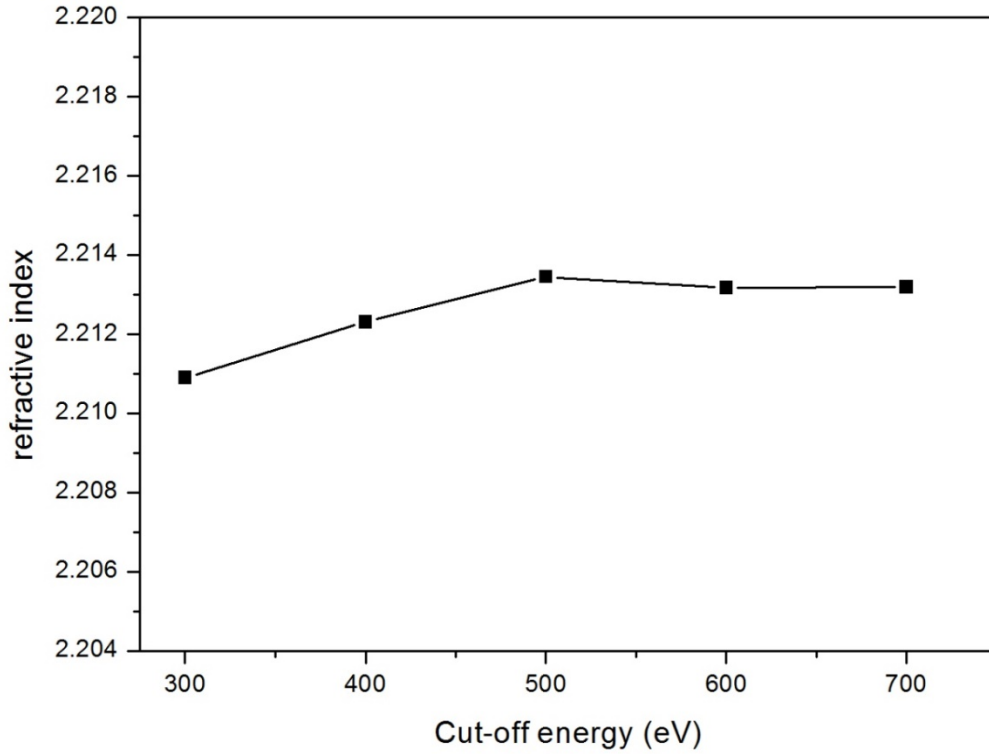
CASTEP Optical Properties
Scissors operator = 0 eV, Instrumental smearing : 0.5 eV
Calculation geometry: Polarized, polarization direction: (0.000 0.000 1.000)



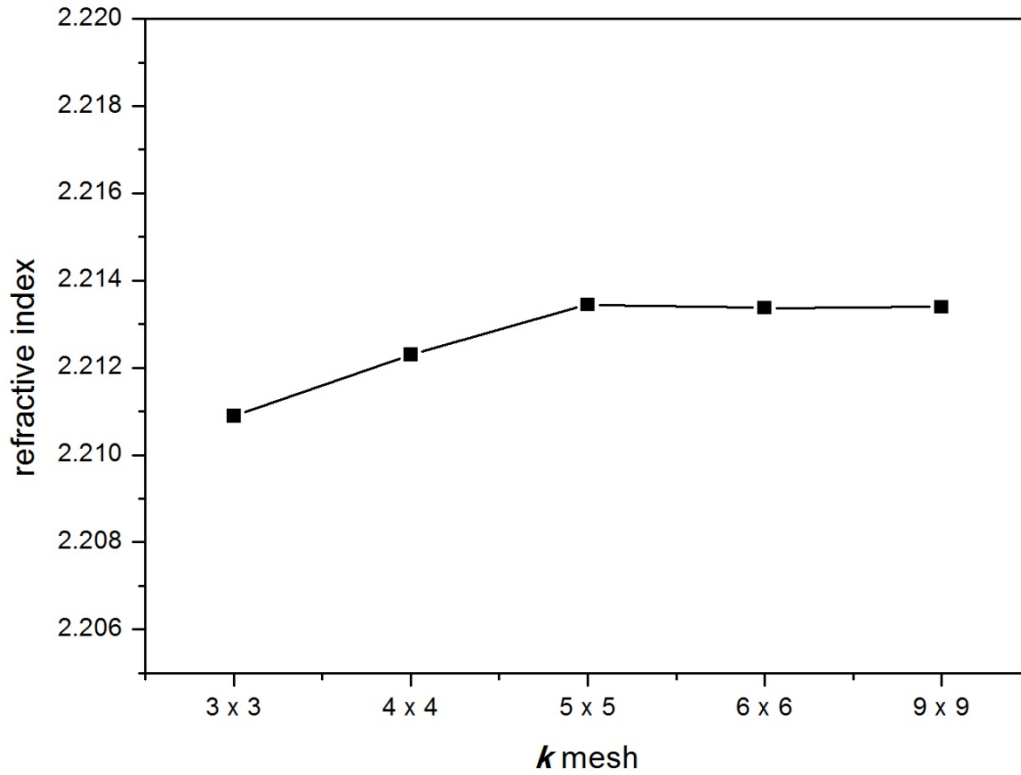
S 3. real and imaginary part of Refractive index along 001 direction

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 (4x4) 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.