Poster Presentation

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Polymerization of acrylamide under high pressure: a first-principles study

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Abstract:

The study of materials under pressure have gained tremendous interest in recent times because it can provide unique structural and dynamical properties not seen under ambient conditions.[1,2,3] We present our recent DFT study on solid state polymerization under hydrostatic pressure for acrylamide ($P2_1/c$) having intra-dimer and inter-dimer N-H$^{\cdots}$O bonds. Our detailed analysis reflects the effect of pressure on energy landscape of chemical reaction from 0 to 102 GPa by using PBE+vdW functional. We have found two different stable polymeric structures ($P\bar{1}$, $P2_1/c$) through two different pathways in potential energy surface which is primarily monitored by hydrogen bonding distortions. Detailed investigations on dynamic stability and normal mode analysis of different structures under a wide pressure range indicate good correlation with experimental IR and Raman analysis. The mechanism of polymerization is confirmed by spin density and Löwdin charge analysis as well as electronic band structure calculations.

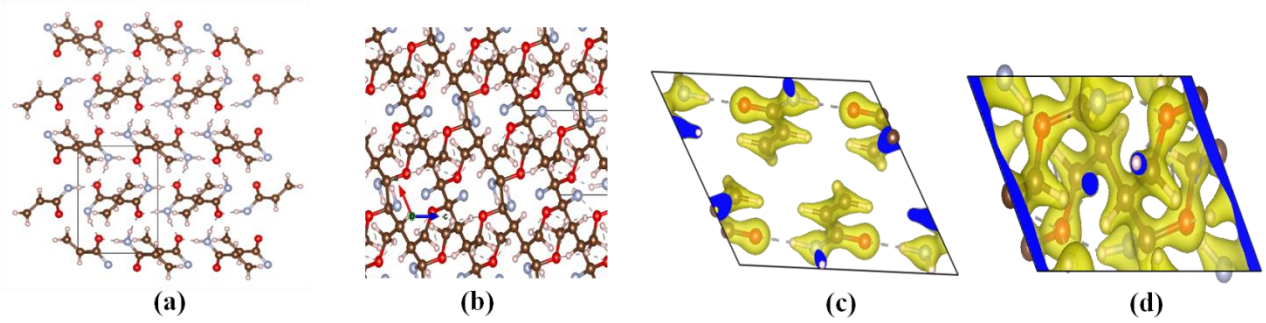

Figure: (a) Acrylamide at 0 GPa (b) Polymer chain at102 GPa via C-C/ C-O bonds formation Charge density plots (isosurface value 0.2): At (c) 0 GPa and (d) 102 GPa

References:

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