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BOOK OF ABSTRACTS

Radiation effects in spatially confined amorphous pnictochalcogenides: A computational insight through cluster modeling code CINCA

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Phenomenology of radiation induced effects in amorphous pnictochalcogenides A_xB_{1-x} (where pnictogen A = P, As, Sb, Bi; and chalcogen B = S or Se) is critically reexamined with respect to intrinsic free volume available for their realization. Destruction of covalent chemical bonds in these alloys under above bandgap irradiation is accompanied by relaxation in a new structural state. When such relaxation occurs via switching of heteronuclear (A-B) bonds into homonuclear (A-A) and (B-B) ones, like under intrinsic decomposition in amorphous stoichiometric $As_2(S/Se)_3$, an additional volume appears resulting in a red shift of optical absorption edge. Assuming that double-bond based $B=As(B_{1/2})_3$ units are stabilized due to inner pressure because of nanoconfined spatial geometry, a blue shift is expected. This analysis based on ab-initio quantum-chemical modeling of atomic clusters clarify misunderstanding with double bond based $B=As(B_{1/2})_3$ units as principal structural species facilitating self-organization in binary pnictochalcogenide A-B compounds.