

## عنوان مقاله:

(Polarizability and second hyperpolarizability of  $M@B_2F_{12}N_2$  cages (M=Li, Na and K

## محل انتشار:

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## خلاصه مقاله:

By applying B<sup>3</sup>LYP/6-31G\* time dependent density functional level of theory and sum-over-state (SOS) approach, the static and frequency dependent polarizability and second hyperpolarizability properties of the , , and cages have been studied. The polarizability and second hyperpolarizability properties of cage have been studied by considering effects of Li, Na and K atoms encapsulation in the cage. The type and encapsulation of M atom can greatly impress on polarizabilities and second hyperpolarizabilities values of cage. As, highest peak value of second hyperpolarizabilities for is about ۲۳ times larger than that of the , and cages. It seems that cages can be used to produce the semiconductors with various band gaps

## کلمات کلیدی:

Ab initio, B-N Material, Cage, Density Functional, Endoedral, Sum-over-state

## لینک ثابت مقاله در پایگاه سیویلیکا:

<https://civilica.com/doc/1455504>

