

## عنوان مقاله:

Quantification of local  $\sigma$ - $\pi$  mixing in bent conjugated systems: application to C60 buckminsterfullerene

## محل انتشار:

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## خلاصه مقاله:

The circular curvature of carbon atoms in carbon nanotubes and fullerenes avoids highest possible overlap between perpendicular p orbitals and categorizes them as interesting systems [1]. This curvature also affects the properties associated with the  $\pi$  system, such as aromaticity. In the present work, we aim to get deeper insight into the nature of  $\sigma$  and  $\pi$  systems of fullerene and quantify their local mixing. Natural bond orbitals (NBO) [2] will be used to prepare orthogonalized  $\sigma$  and  $\pi$  systems.

## کلمات کلیدی:

لینک ثابت مقاله در پایگاه سیویلیکا:

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