عنوان مقاله:

Electrostatic and symmetry control on the accuracy of molecular orbital diagram forecasts: A double hybrid DFT calculation

محل انتشار:

هفتمین کنگره ملی شیمی و مهندسی شیمی با تاکید بر فناوری های بومی ایران (سال: 1399)

تعداد صفحات اصل مقاله: 7

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خلاصه مقاله:

This work provides a comprehensive computational study on the limitations of molecular orbital theory for predictingthe behavior of systems. In this investigation, the quantum chemical calculations were used. All density functionaltheory calculations were carried out employing the double-hybrid method of Grimme's B2PLYP combined withGrimme's D3BJ dispersion and with the basis set of 6-31++G(3df, 3pd). The results obtained clearly indicate thefailure of molecular orbital theory in special conditions. In these situations, the results are not consistent with reality.This inconsistency can be attributed to the strong electrostatic fields and can be corrected by using the .stabilizers ofthese fields

کلمات کلیدی:

Molecular orbital theory, Electrostatic and symmetry control, Computational insights