

Comparative Study of the Therapeutic Potential of C₂₄, C₃₂, B₁₂N₁₂, and B₁₆N₁₆ Nanocages as Drug Delivery Carriers for Delivering an Erlotinib Derivative: DFT and QTAIM investigations

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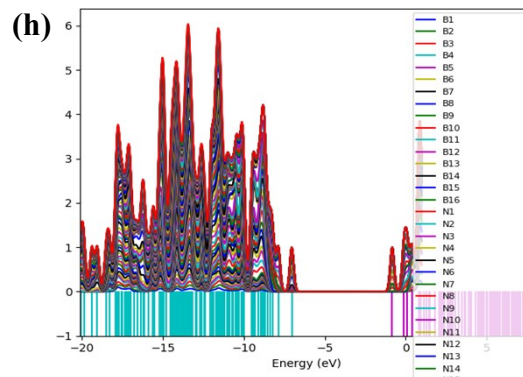
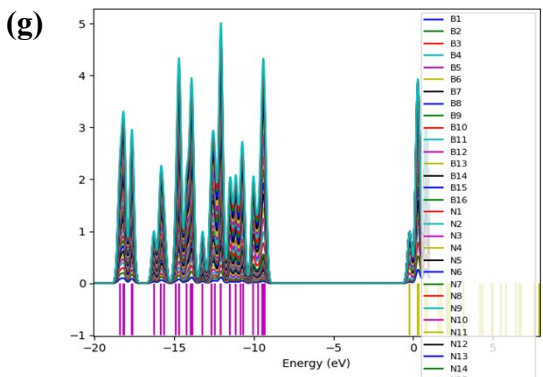
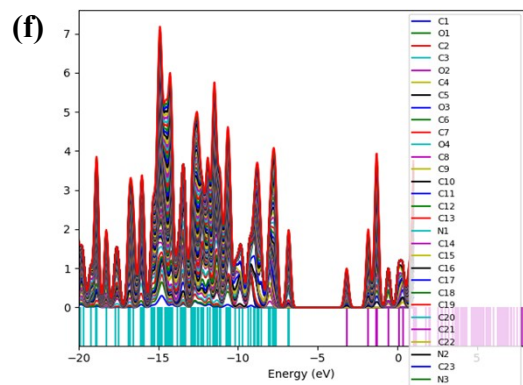
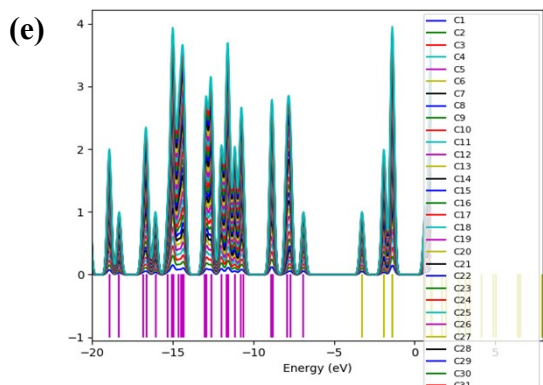
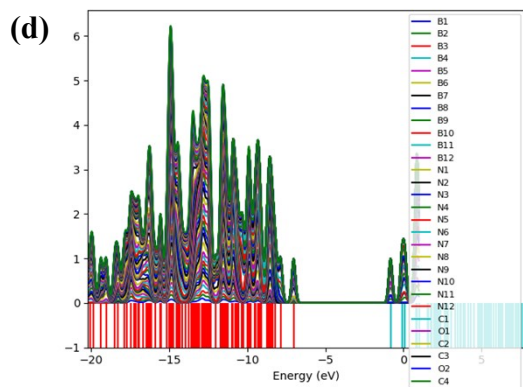
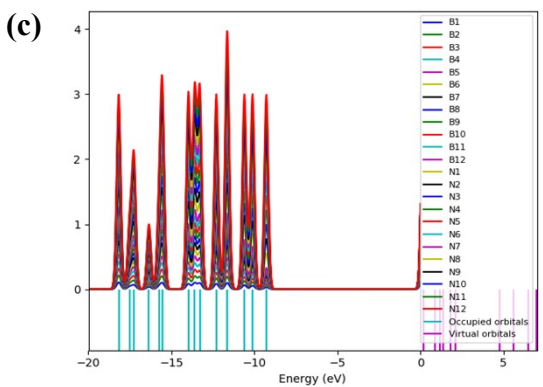
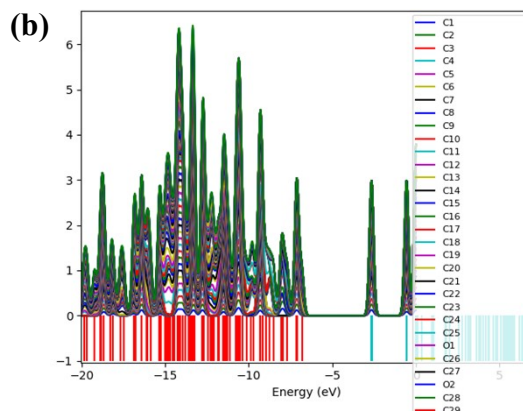
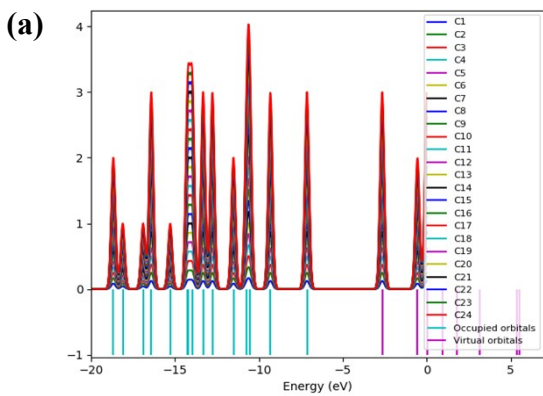


Fig. S1. PDOS plot shows the atoms involved in the intermolecular interactions of the energetically favorable methylerlotinib on C₂₄ nanocage, (b) methylerlotinib@C₂₄-nanocage, (c) B₁₂N₁₂-nanocage, (d) methylerlotinib@B₁₂N₁₂-nanocage, (e) C₃₂-nanocage, (f) methylerlotinib@C₃₂-nanocage, (g) B₁₆N₁₆-nanocage, and (h) methylerlotinib@B₁₆N₁₆-nanocage.