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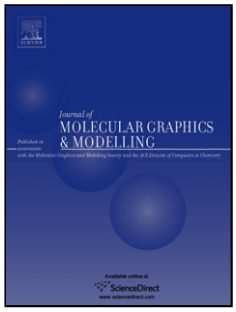

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ACCEPTED MANUSCRIPT

Theoretical Study on Electron Structure and Charge Transport Properties of Tetraazapentacene Derivatives

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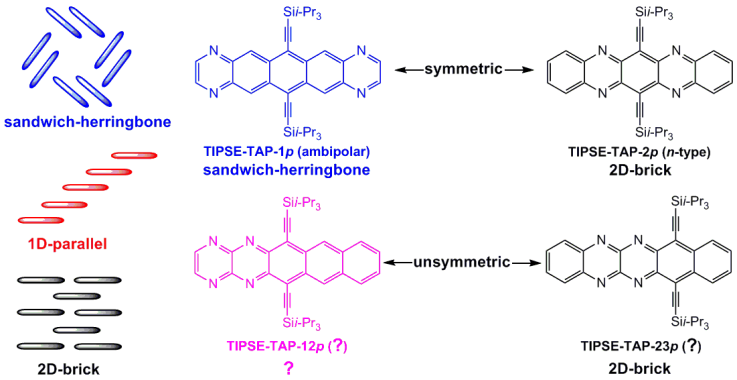
Graphical abstract



Highlights

- The unsymmetric tetraazapentacene derivatives have lower LUMO levels to facilitate electron injection.
- The reorganization energy of tetraazapentacene derivatives is small and not very sensitive to the position of four nitrogen atoms.
- The π···stacking is more beneficial for electron transport of tetraazapentacene derivatives.
- The tetraazapentacene derivatives have a three-in-one advantage for electron transport.

Abstract: By Means of Marcus electron transfer theory, the charge transport properties of tetraazapentacene (**4N-PEN**) derivatives were systematically explored. The reorganization energies were studied by both adiabatic potential-energy method and normal mode analysis. The charge diffusion constants were evaluated from the random walk simulation. From the perspective of homology modeling, a selected **4N-PEN** derivative without experimental crystal structure was

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