Supporting Information

A DFT analysis of the ground and excited states electronic structure of $Sc_3N@I_h$-C_{80} fullerene coupled with metal-free and zinc-phthalocyanine

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TABLE I: The numbers of s-, p-, d-type contracted functions, number of primitive gaussians and the range of the gaussian exponents used for each atom.

Atom	s-type	p-type	d-type	Primitives	Exponent range
C	5	4	3	12	$2.22 * 10^4$- 0.077
H	4	3	1	6	7.78 * 10 - 0.074
N	5	4	3	13	$5.17 * 10^4$- 0.094
Sc	7	5	4	19	$156.52 * 10^4$- 0.035
Zn	7	5	4	20	$500.8 * 10^4$ - 0.055

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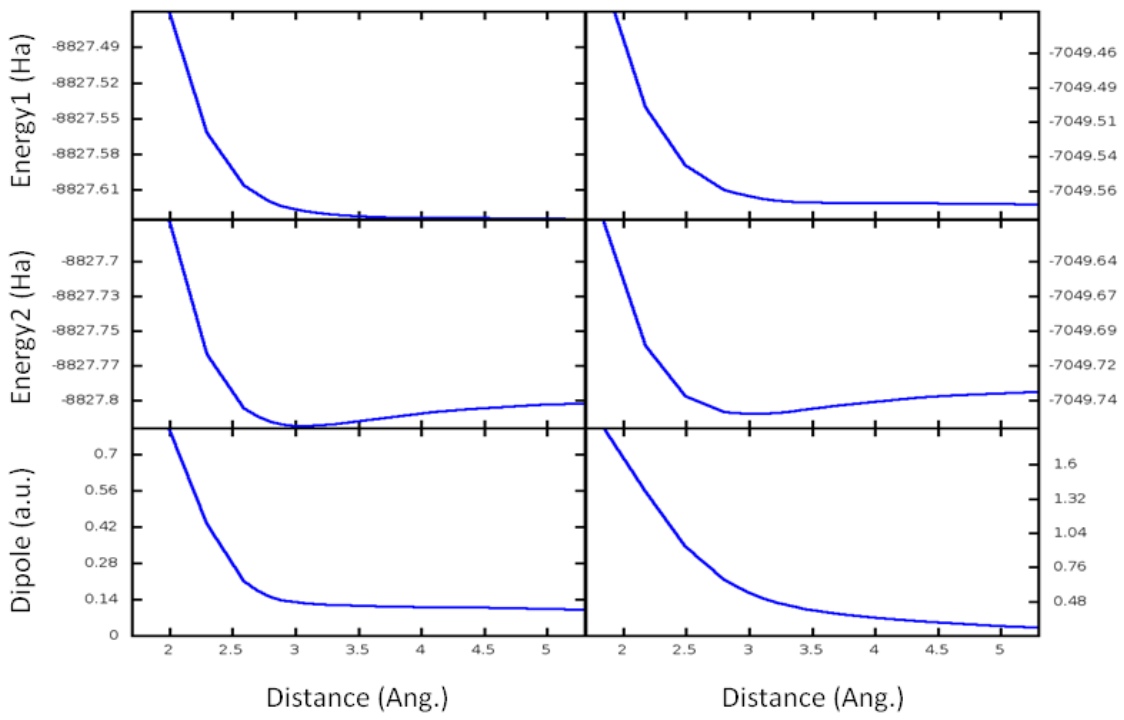

FIG. 1. The ground state dipole moments and total energies as a function of donor-acceptor separation in $Sc_3N@C_{80}$-ZnPc (left panels) and $Sc_3N@C_{80}$-H_2Pc (right panels) dyads. In Energy1 values, the dispersion energy is not included while in Energy2 values, it is taken into account.

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