Electronic Supplementary Information for "Aromaticity, Coulomb repulsion, π delocalization or strain: who is who in endohedral metallofullerene stability?"

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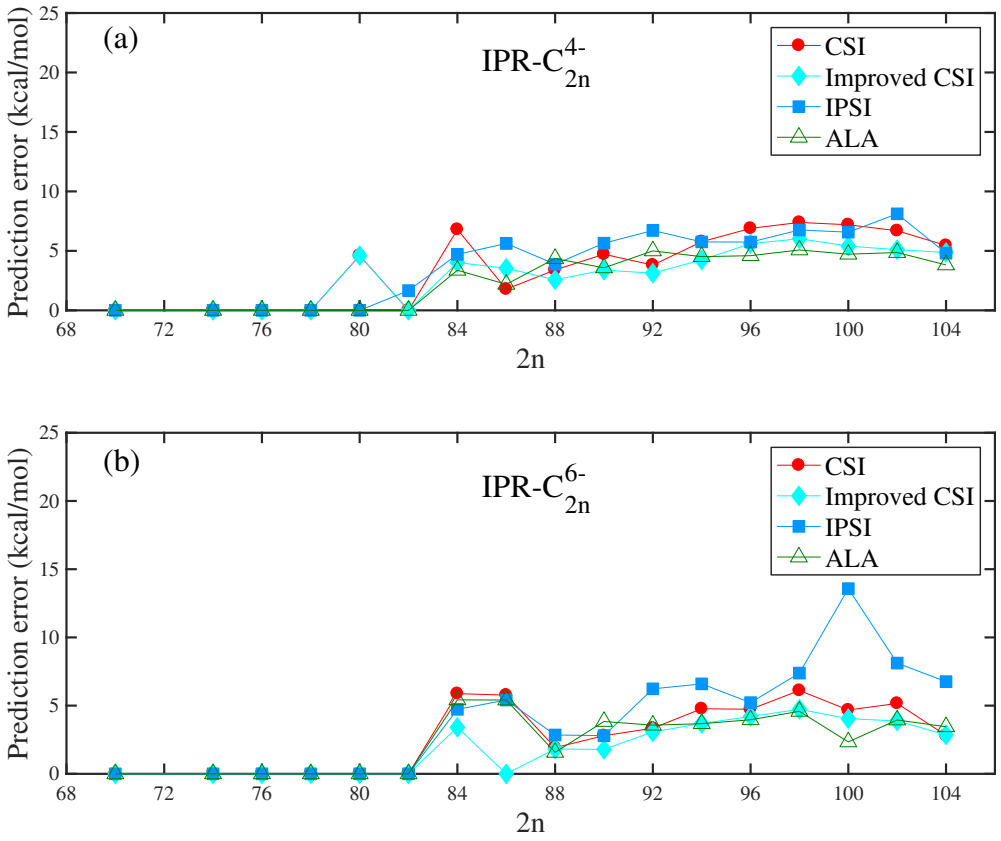

Figure S1. Prediction error for the CSI (red circles), improved CSI (cyan diamonds), ALA (green triangles) and IPSI (blue squares) models for the IPR fullerene anions (a) C_{2n}^{4-} and (b) C_{2n}^{6-}, with cage sizes $2n = 70$–104.

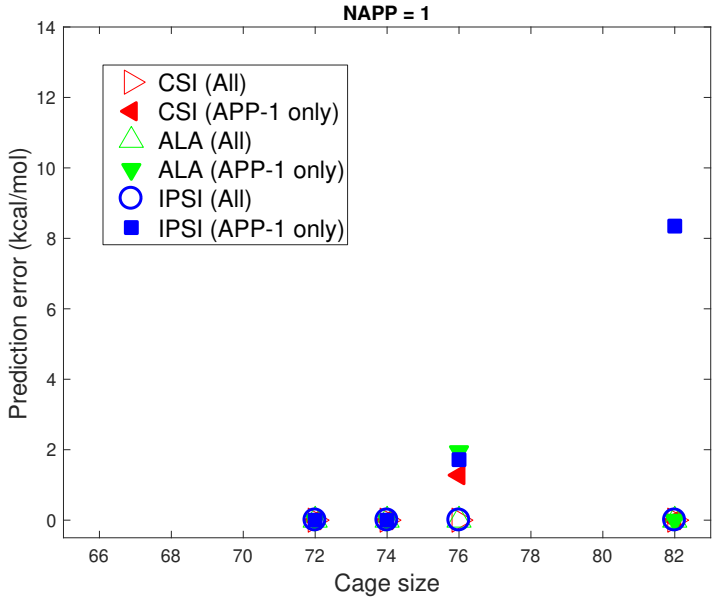

Figure S2. Prediction error for the indicators CSI, ALA and IPSI for fullerene anions C_{2n}^{6-} ($2n$ = 66–82). Empty symbols correspond to the prediction error calculated by including all non-IPR isomers (with up to 3 APPs), whose relative energy is lower than 30 kcal/mol. Filled symbols represent the prediction error calculated by considering only the isomers with one APP, within the 30 kcal/mol window. The reference energy of the latter is that of the most stable one among all isomers with one APP.

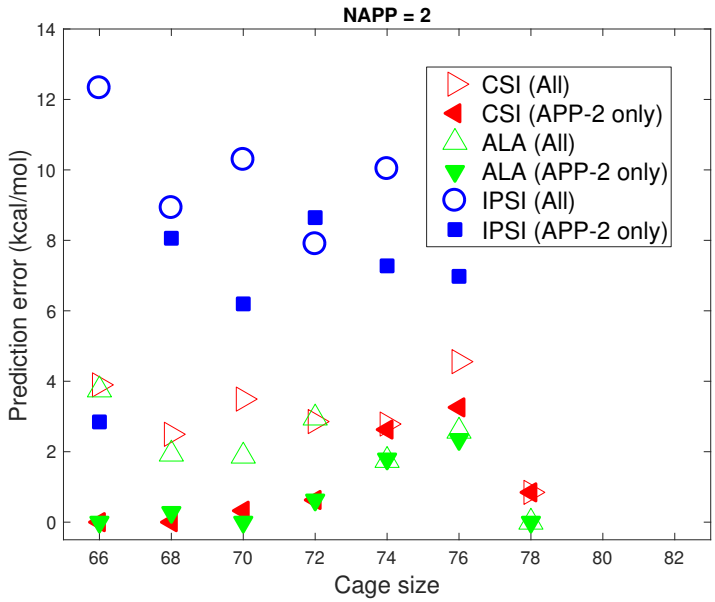

Figure S3. Prediction error for the indicators CSI, ALA and IPSI for fullerene anions C_{2n}^{6-} ($2n$ = 66–82). Empty symbols correspond to the prediction error calculated by including all non-IPR isomers (with up to 3 APPs), whose relative energy is lower than 30 kcal/mol. Filled symbols represent the prediction error calculated by considering only the isomers with 2 APPs, within the 30 kcal/mol window. The reference energy of the latter is that of the most stable one among all isomers with 2 APPs.

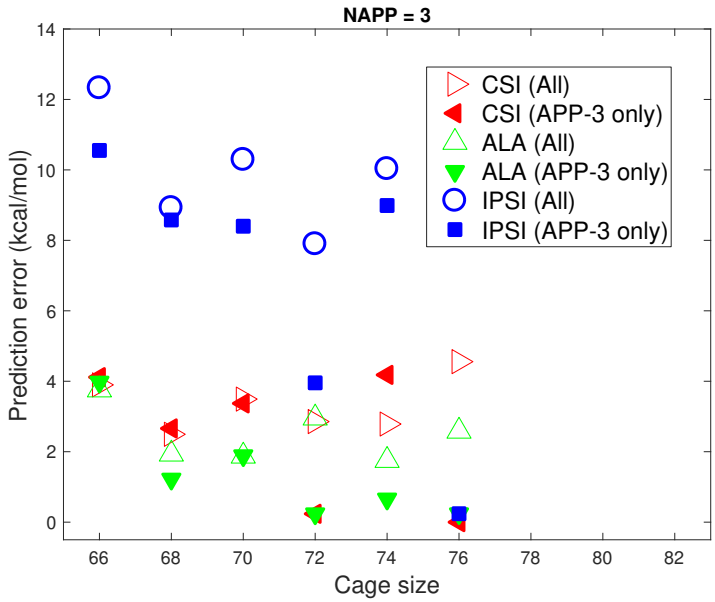

Figure S4. Prediction error for the indicators CSI, ALA and IPSI for fullerene anions C_{2n}^{6-} ($2n$ = 66–82). Empty symbols correspond to the prediction error calculated by including all non-IPR isomers (with up to 3 APPs), whose relative energy is lower than 30 kcal/mol. Filled symbols represent the prediction error calculated by considering only the isomers with 3 APPs, within the 30 kcal/mol window. The reference energy of the latter is that of the most stable one among all isomers with 3 APPs.