## Structures and Energetics of Neutral and Cationic Pyrene Clusters Supplementary Materials

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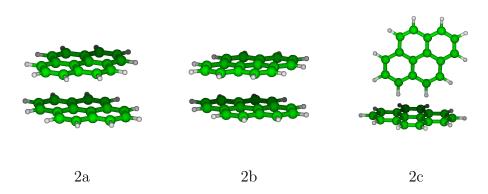


Figure S1: most stable structures for neutral pyrene dimers

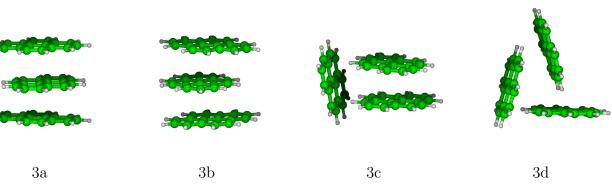


Figure S2: most stable structures for neutral pyrene trimer

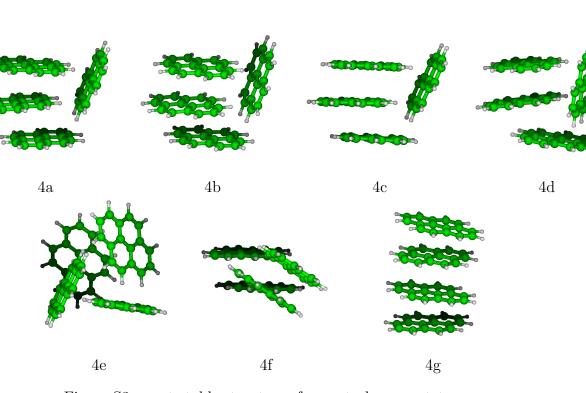


Figure S3: most stable structures for neutral pyrene tetramer

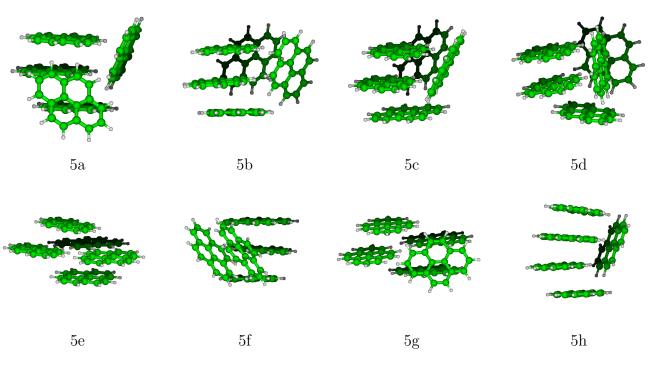


Figure S4: most stable structures for neutral pyrene pentamer

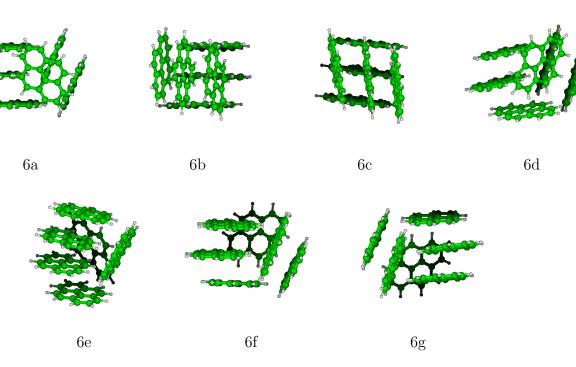


Figure S5: most stable structures for neutral pyrene hexamer

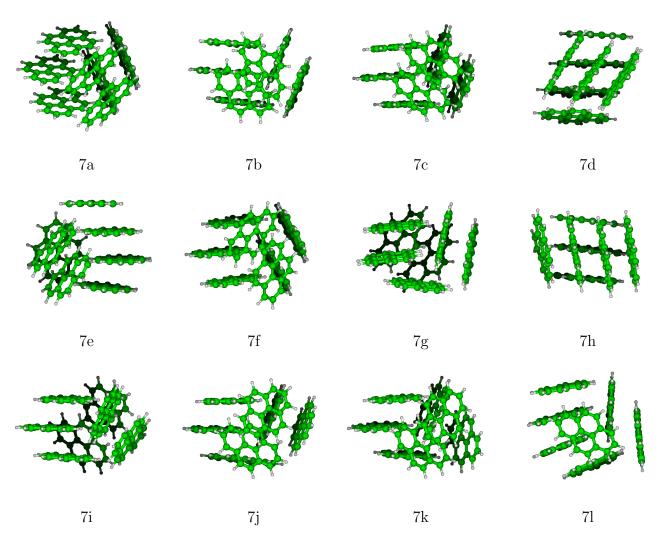


Figure S6: most stable structures for neutral pyrene heptamer

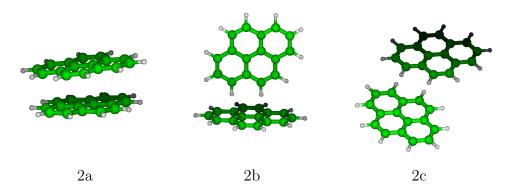


Figure S7: most stable structures for cationic pyrene dimers

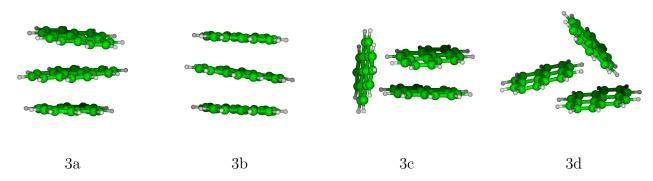


Figure S8: most stable structures for cationic pyrene trimer

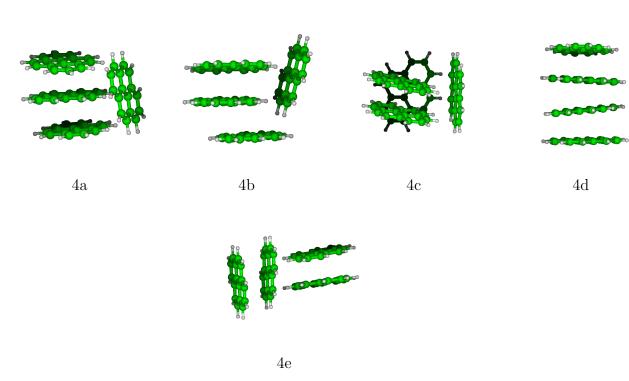


Figure S9: most stable structures for cationic pyrene tetramer

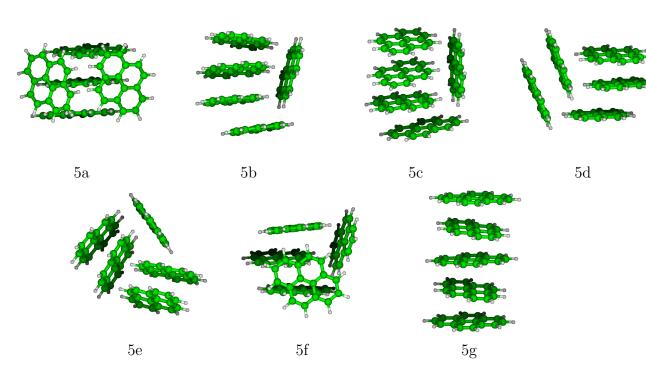


Figure S10: most stable structures for cationic pyrene pentamer  $\,$ 

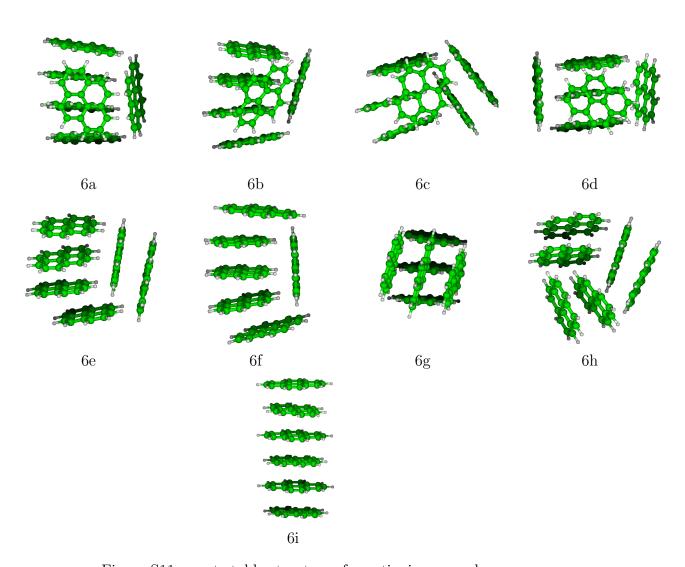


Figure S11: most stable structures for cationic pyrene hexamer

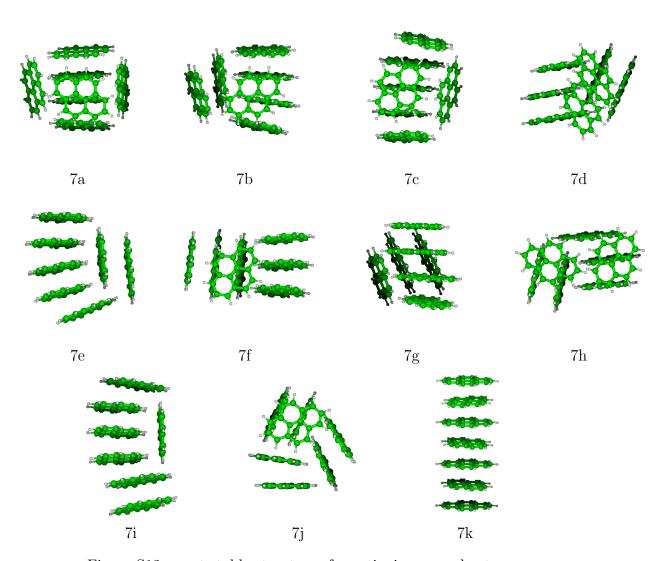


Figure S12: most stable structures for cationic pyrene heptamer