

SUPPLEMENTARY MATERIALS

Methodological investigation for hydrogen addition to small cage carbon fullerenes

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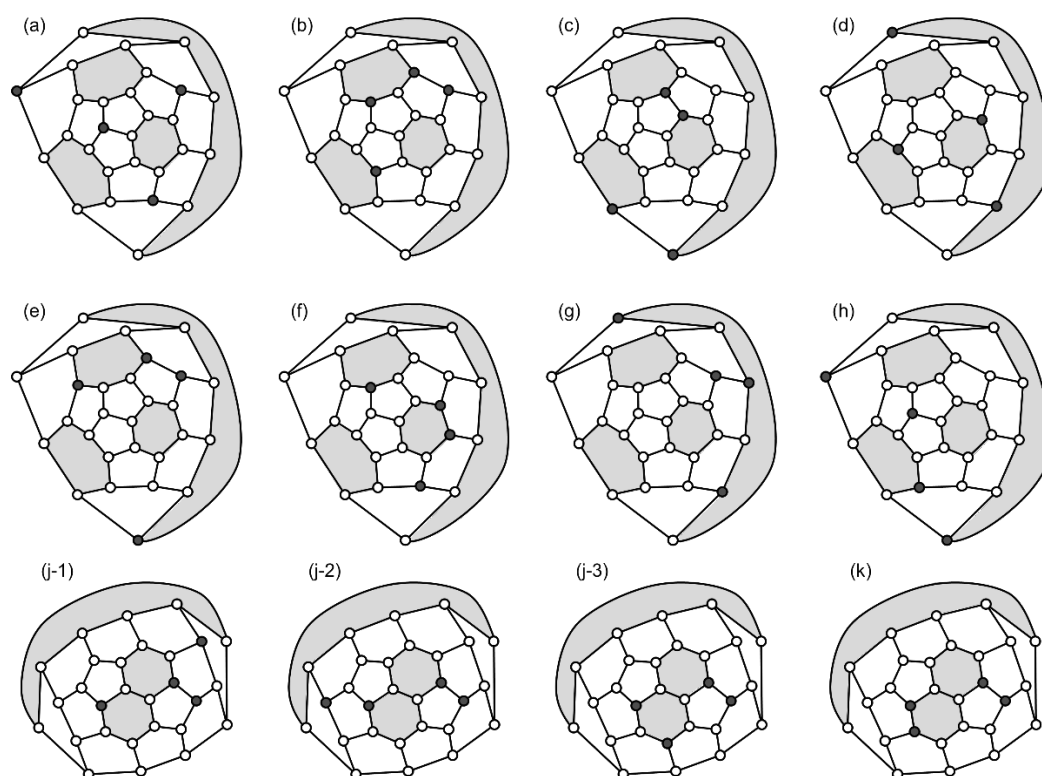


Figure S1. Schlegel projections of optimal $C_{28}H_4$ structures obtained by (a) GFN2-xTB all combination test, PM7, PM6+D3, RM1, GFN2-xTB, and sequential all sites testing by DFT, (b) hybridisation value and pyrA, (c) 2 bond lengths sum and 3 bond lengths sum, (d) Mulliken value, (e) minimum frontier value with 0.1e addition, (f) minimum frontier orbital value with 1e addition, (g) maximum frontier value with 0.1e addition, (h) maximum frontier value with 1e addition, (i) AIREBO, (j) REBO, (k) AIREBO-M. For (j), there are three structures with the same energy within calculation error. White circles indicate carbon atoms, dark circles show hydrogenated carbons. Hexagons are shaded in grey, for the D_2 -symmetry cage (j-k) the fourth hexagon is that surrounding the plot.

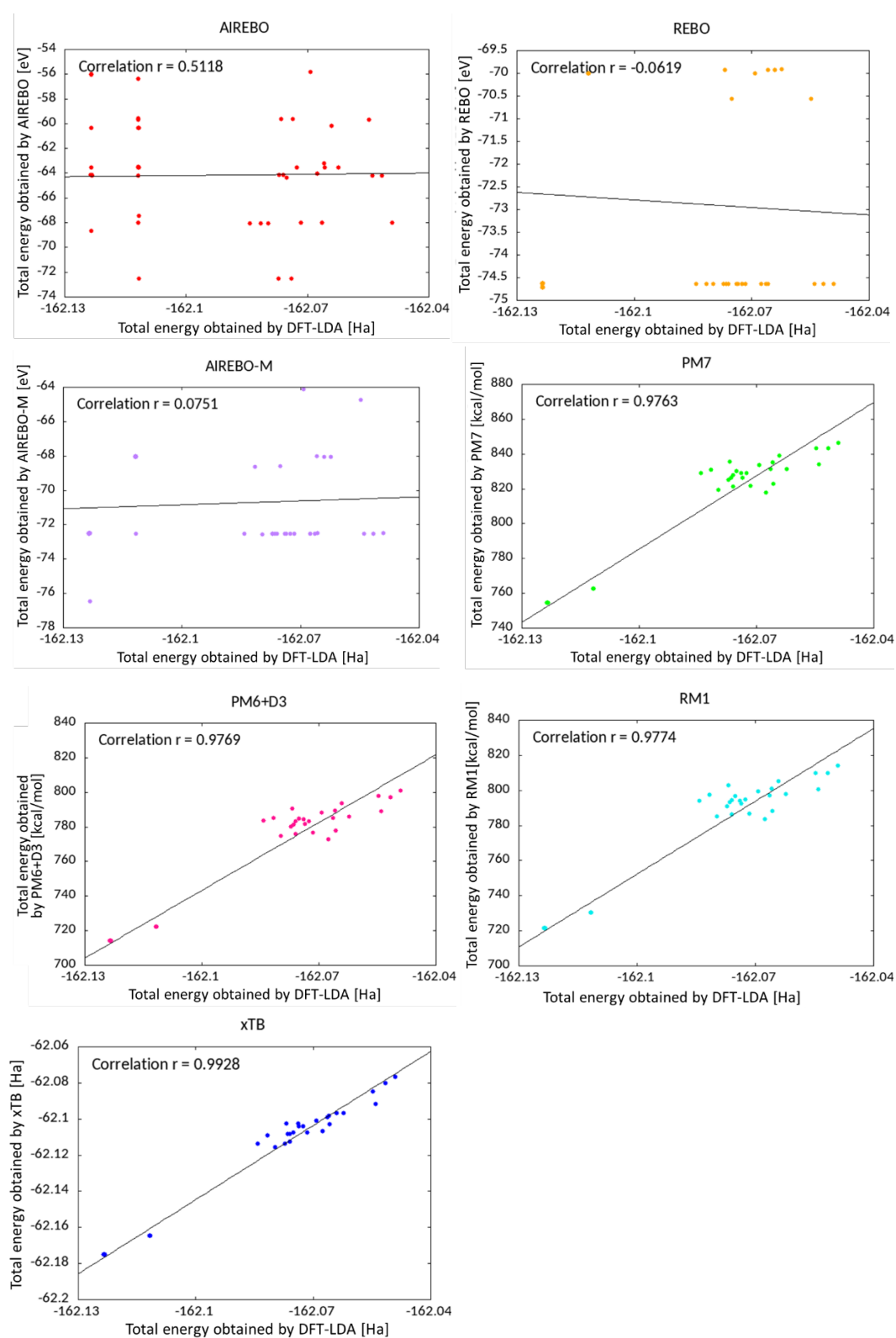


Figure S2. Total energy correlation plots for isomers of $C_{28}H_5$. Energy obtained by DFT-LDA is plotted along the x-axis and by empirical and semi-empirical methods along the y-axes as labelled. Linear correlation in each model is shown as r in each plot.

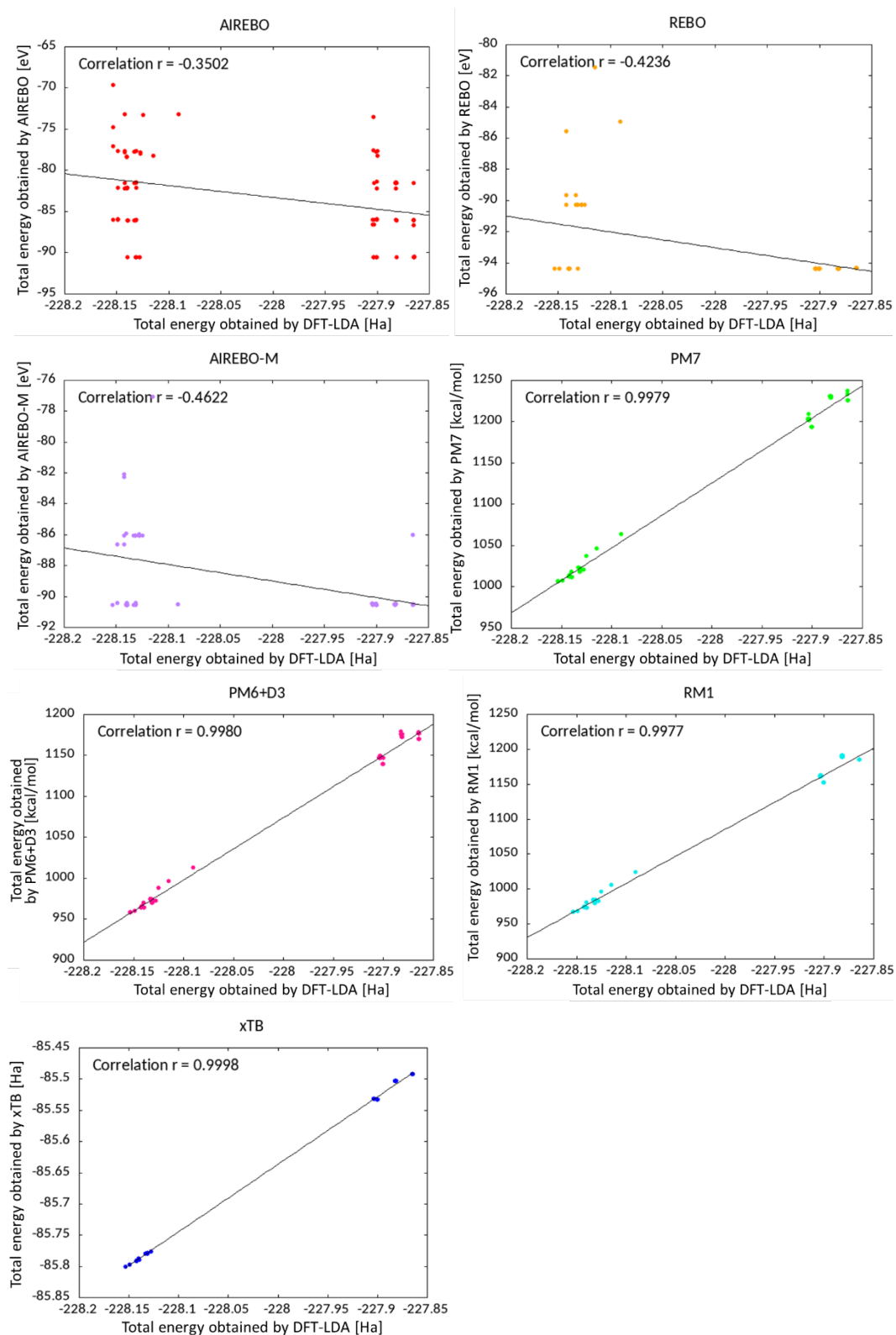


Figure S3. Total energy correlation plots for isomers of $C_{40}H$. Energy obtained by DFT-LDA is plotted along the x-axis and by empirical and semi-empirical methods along the y-axes as labelled. Linear correlation in each model is shown as r in each plot.