Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Effect of Fluoro and Hydroxy Analogies of Diglyme on Sodium-Ion Storage in Graphite: A Computational Study

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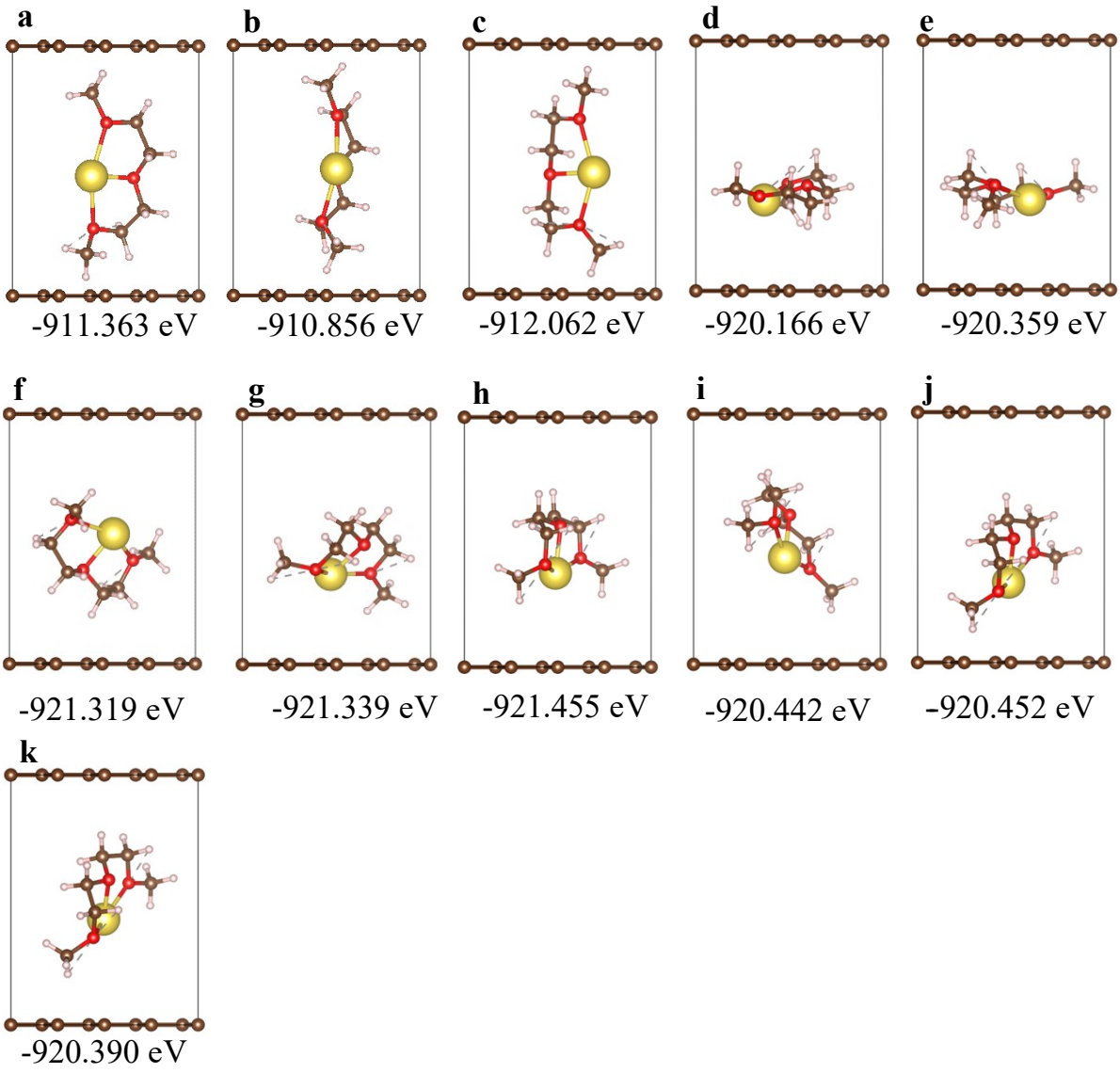


Fig. S1 Initial configurations used to identify the most stable structure for D_2-G system.

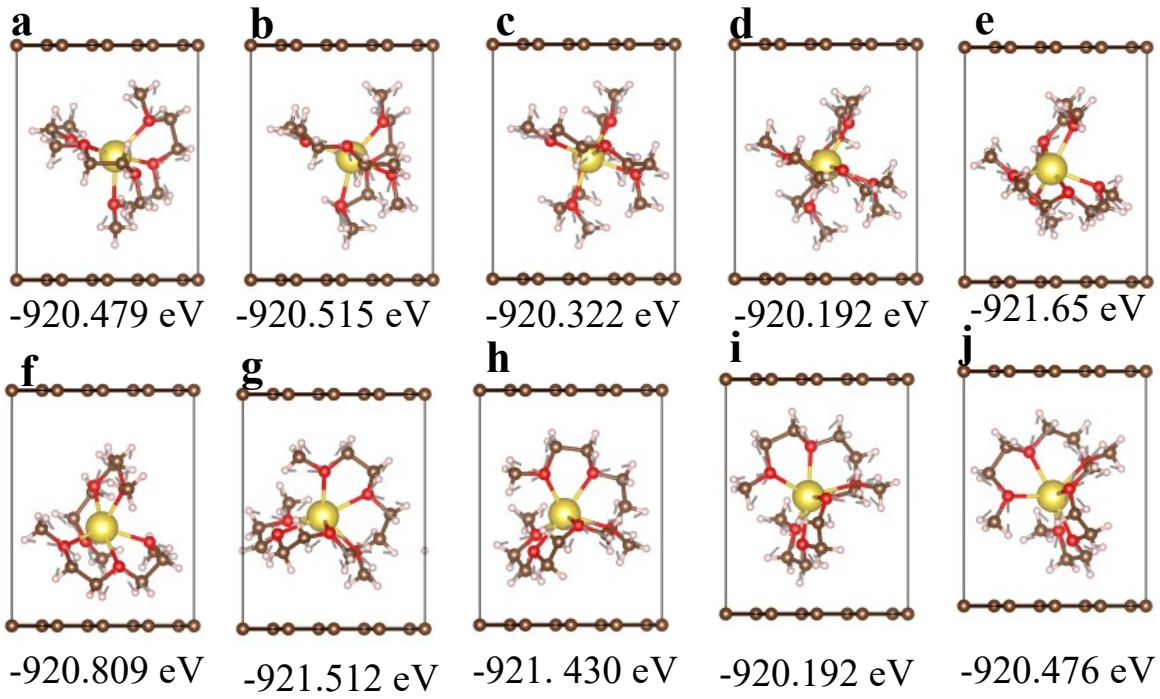


Fig. S2 Initial configurations used to identify the most stable structure for D_1-G system.

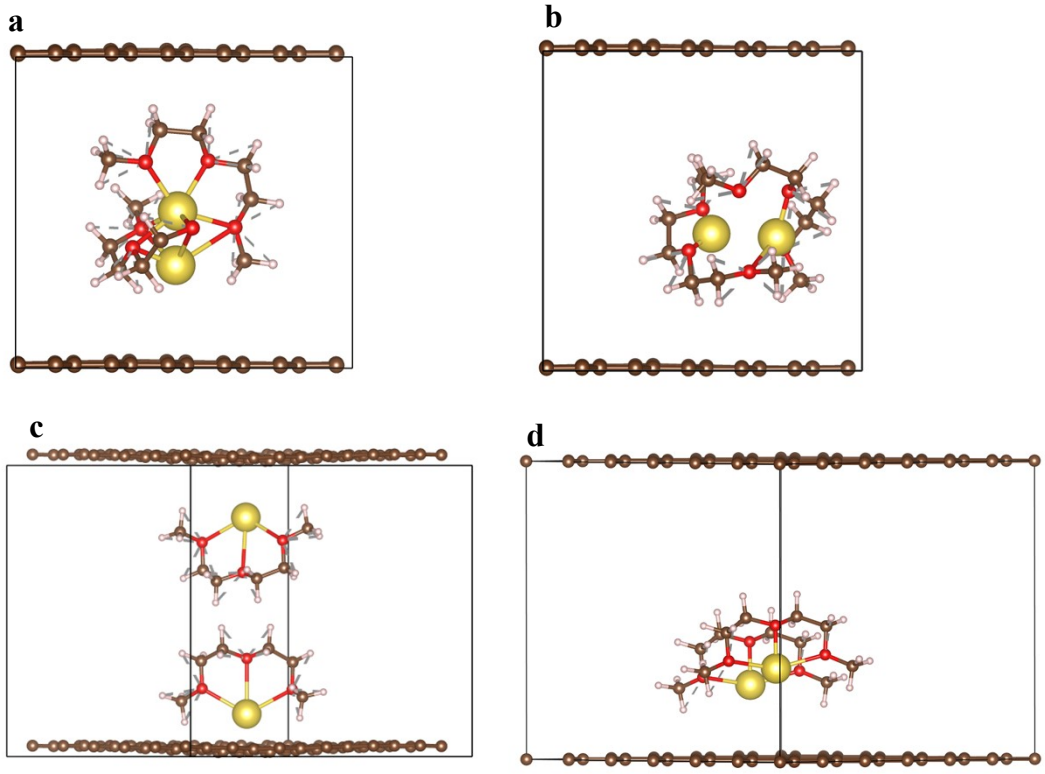


Fig. S3 Four different initial configurations used for the calculation of Na_2-D_2-G system. Energies are a) -922.11 eV b) -922.15 eV c) -922.27 eV and d) -922.21 eV, respectively.

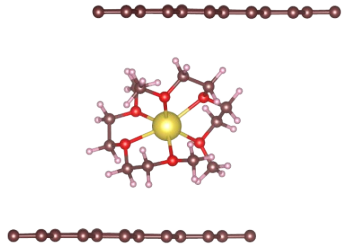
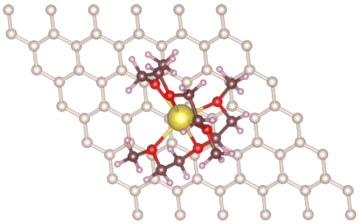
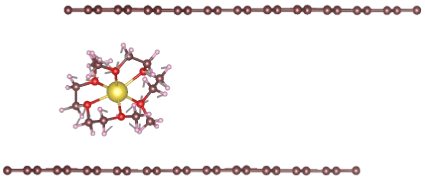
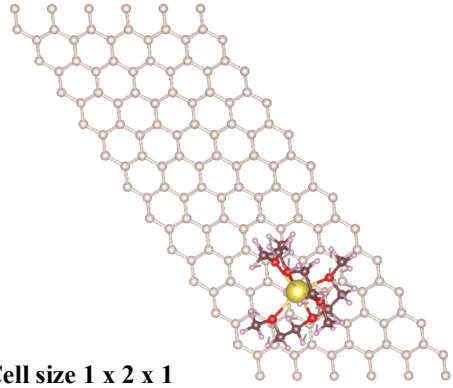
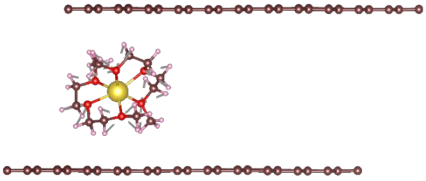
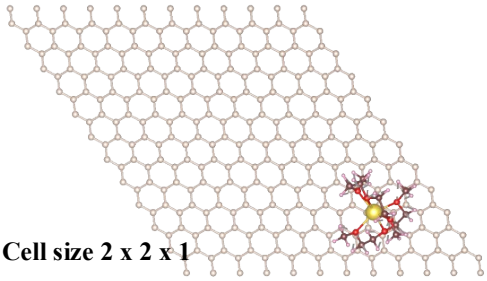
Side view	Top view	Binding Energy
	 Cell size 1 x 1 x 1	-3.498 eV
	 Cell size 1 x 2 x 1	-3.614 eV
	 Cell size 2 x 2 x 1	-3.726 eV

Fig. S4 Calculated binding energy for the increased unit cell sizes. The initial unit cell size has been increased along the a and b direction to study the binding energy change when increasing the unit cell size.