**Supplementry Information**

**Adsorption of an Azo Dye on Graphene Nanosheet: A Molecular Dynamics Simulation Study**

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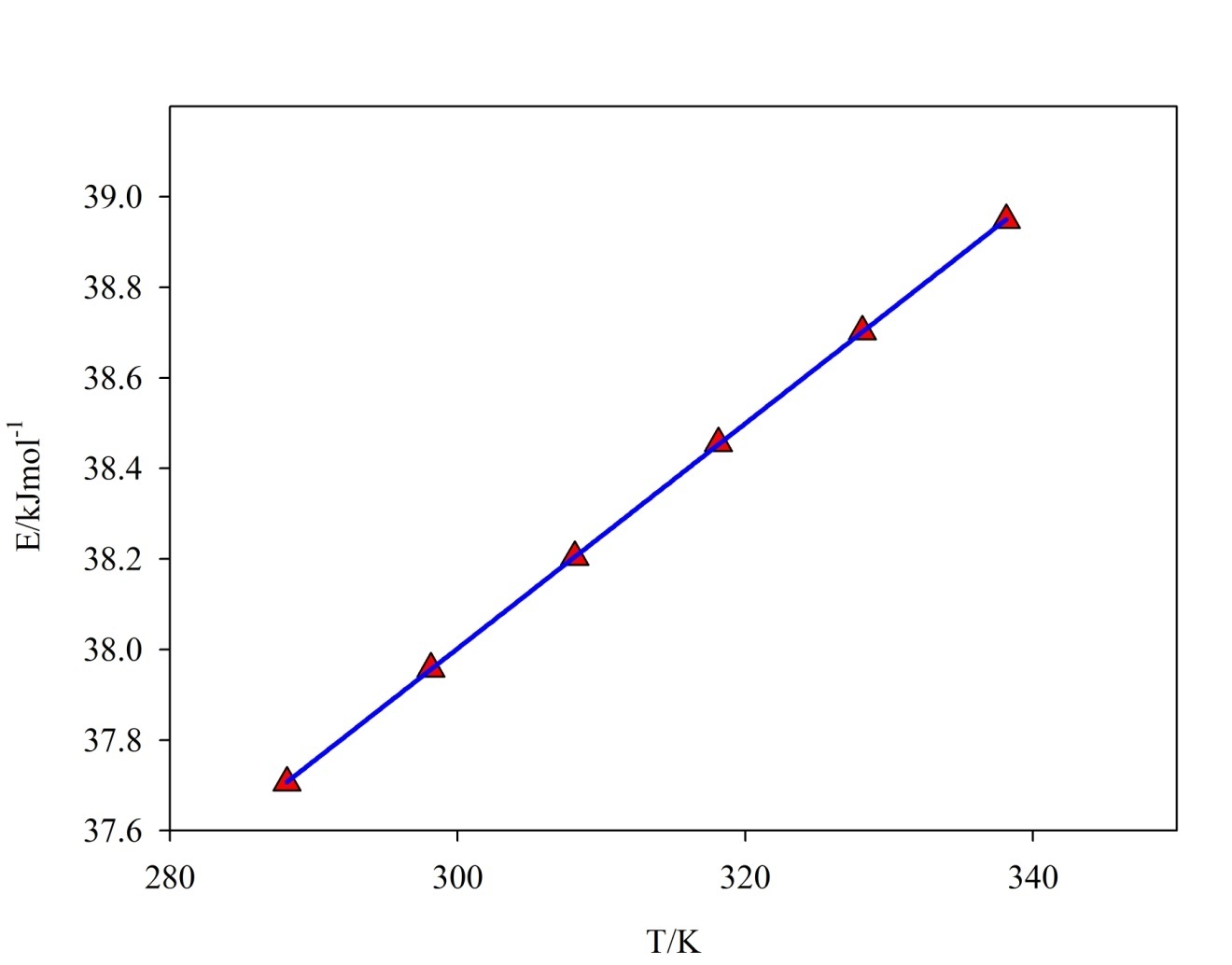
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**Table S1.** Structural parameters for the ground state of dye calculated at B3LYP/6-31+G\* level of theory. Labels for atoms can be found in Fig. 1.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Bond length/Å | | Bond angle/degree | | Atomic charge/C | |
|  | N1-C2 1.41733  C2-C3 1.40728  C3-C5 1.39310  C5-C9 1.39765  C7-C9 1.39905  C4-C7 1.39247  C4-H8 1.08500  C7-H11 1.08591  C5-H10 1.08566  C3-H6 1.08883  C9-S12 1.80303  S12-O13  1.47493  S12-O14 1.47529  C15-H16 1.09368  C15-H70 1.09362  C61-H63 1.09491  C61-H62 1.09482  C61-O64 1.43490  O64-S65 1.65955  S65-O67 1.50816  S65-O66 1.50808  S65-O68 1.45397  S65-Na69 2.75558  N17-C25 1.37570  C25-C26 1.43689  C26-S56 1.83220  S56-O58 1.50366  O59-S56 1.50507  S56-O57 1.46738  S56-Na60 2.74168  C23-C26 1.38098  C23-H27  1.08476  C23-C20 1.41939  C20-C21 1.40486  C21-C24 1.38081  C24-C25 1.43523  C24-O29 1.35059  O29-H30 0.98573  C19-C20 1.42795  C19-H28 1.08429  C21-N31 1.46916  N31-H32 1.03768  N31-H33 1.03485  N31-C22 1.50258  C18-C22 1.41482  C18-C19 1.37356  C22-N34 1.31860  C18-S51 1.83612  S51-O52 1.46554  S51-O53 1.50366  S51-O54 1.50096  S51-Na55 2.77007  N34-N35 1.31709  N35-C36 1.39544  C36-C37 1.41066  C37-H40 1.08605  C37-C39 1.39001  C39-H44 1.08594  C39-C43 1.40128  C41-C43 1.39782  C38-C41 1.39375  C36-C38 1.41669  C38-H42 1.08784  C41-H45 1.08633  C43-S46 1.79700  S46-O47 1.47651  S46-O48 1.47448  S46-C49 1.82519  C49-H50 1.09362  C49-H80 1.09389  C49-C71 1.52603  C71-H73 1.09460  C71-H72 1.09315  C71-O74 1.44374  O74-S75 1.66105  S75-O76 1.46111  H75-O78 1.49882  S75-O77 1.50840  S75-Na79 2.73924 | O66-S65-O67 107.330  S65-O64-C61 116.616  C61-C15-S12 110.194  O13-S12-O14 120.811  C15-S12-C9 103.671  S12-C9-C5 119.271  C9-C5-C3 119.046  C5-C3-C2 120.440  C3-C2-C4 119.718  C2-C4-C7 119.975  C4-C7-C9 119.523  C2-N1-N17 113.284  N1-N17-C25 124.689  N17-C25-C26 134.623  C25-C26-S56 125.465  C25-S56-O57 105.353  C25-S56-O58 105.574  C25-S56-O59 104.553  O57-S56-O58 115.245  S56-C26-C23 114.311  C26-C23-C20 122.906  C23-C20-C21 116.706  C20-C21-C24 122.070  C21-C24-C25 121.406  C21-C24-O29 117.422  C24-O29-H30 105.397  C24-C21-N31 117.590  C21-N31-C22 116.110  N31-C22-C18 118.003  C22-C18-C19 122.513  C22-C18-S51 118.809  C18-S51-O53 103.156  O54-S51-O52 116.518  C22-N34-N35 115.981  N34-N35-C36 113.205  N35-C36-C38 123.407  N35-C36-C37 117.801  C36-C37-C39 120.680  C37-C39-C43 119.631  C39-C41-S46 119.788  C43-S46-O47 107.567  C43-S46-O48 107.911  C43-S46-C49 103.960  S46-C49-C71 110.916  C49-C71-O74  106.684  C71-O74-S75 115.908  O74-S75-O78 101.210  O74-S75-O76 107.420  O76-S75-O77 115.503 |  | N1 0.40734  C2 -1.09882  C3 0.23643  C4 -0.07080  C5 0.69881  H6 0.19453  C7 -0.14526  H8 0.21103  C9 -1.04359  H10 0.23398  H11 0.23635  S12 1.36162  O13 -0.50000  O14 -0.49089  C15 -0.55978  H16 0.27102  N17 -0.71670  C18 -0.53191  C19 -0.07785  C20 1.97315  C21 -1.26422  C22 -0.83357  C23 0.16533  C24 -0.09788  C25 -0.28207  C26 -0.55282  H27 0.26188  H28 0.25945  O29 -0.60141  H30 0.56381  N31 -1.24949  H32 0.54129  H33 0.56539  N34 0.22046  N35 -0.35943  C36 -0.86621  C37 -0.34638  C38 0.55088  C39 0.12367  H40 0.19880  C41 -0.01290  H42 0.21953  C43 -0.85496  H44 0.23001  H45 0.22770  S46 1.32418  O47 -0.48525  O48 -0.46699  C49 -0.43603  H50 0.26657  S51 2.07519  O52 -0.60938  O53 -0.60155  O54 -0.58017  Na55 0.80459  S56 1.80172  O57 -0.58716  O58 -0.60447  O59 -0.64430  Na60 0.79003  C61 -0.27311  H62 0.24311  H63 0.24076  O64 -0.55051  S65 1.67519  O66 -0.78238  O67 -0.78207  O68 -0.58446  Na69 0.86142  H70 0.27066  C71 -0.41451  H72 0.26041  H73 0.24165  O74 -0.58372  S75 1.83888  O76 -0.60875  O77 -0.80281  O78 -0.78317  Na79 0.83048  H80 0.26044 |  |

**Table S2** Structural parameters for the ground state of water calculated at B3LYP/6-31+G\* level of theory.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Bond length/Å | | Bond angle/degree | | Atomic charge/C | |
|  | O1-H2  0.968930  O1-H3 0.968930 | H2-O1-H3 105.505 |  | O1 -0.927570  H2 0.463785  H3  0.463785 |  |



**Fig. S1.** The plot of total energy versus temperature for GNS used for calculation of the isochoric heat capacity.

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