**Supplementry Information**

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

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

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

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