

Interactions between water and dye atoms in the adsorption process of Acid Red-88 on graphene nanosheet: A molecular dynamics simulation

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Water purification is one of the most important environmental concerns because water is directly related to public health, energy production, economic and industrial development. Since dyes are one of the most common environmental pollutants, and are usually toxic, their separation from water resources is very important [1]. This paper contains the results of the adsorption of acid red 88 as a dye from an aqueous solution on graphene nanosurface using molecular dynamics simulation at 298 K by DL_POLY 2.17 software [2].

In this study, the water-dye interactions by use of radial distribution function is analyzed to distinguish which atom of acid red 88 has a stronger interaction with the hydrogen atoms of water molecules and tend to be more hydrophilic. As shown in Figure 1, the greatest interaction between the dye molecule and water hydrogen atoms is from the oxygen side of the sulfite group. In other words, this oxygen atom is more saturated by water molecules than the other atoms which seems to be due to the accumulation of negative loads of oxygen atoms in the part of the dye molecule and increases adsorption of hydrogen atoms by dye. Due to the greater spatial oxygen movement than the dye atoms as well as their number and location, this result is observed.

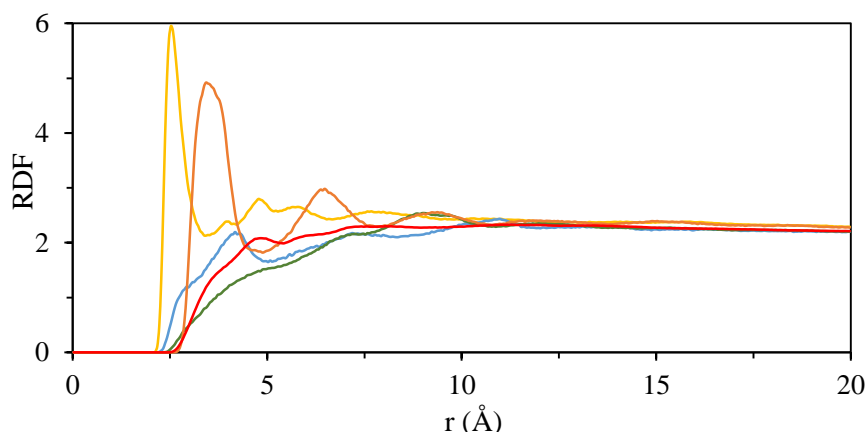


Fig. 1 The RDF plot of dye-water, yellow: oxygen atoms of sulfite group, orange: sulfur atom, blue: oxygen atom of hydroxyl group, green: nitrogen atom, and red: carbon atom.

References

- [1] W. Smith, T. R, Forester, DL_POLY_2. 0: J. Mol, Graphics, **1996**, 14, 136.
 [2] V.K. Gupta, I. Ali, T.A, Saleh, S.Agarwal, RSC Advances, **2012**, 2, 6380.