**Arsenic (As) adsorption studies on functionalized cellulose through molecular dynamic simulation (MDS)**

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Abstract: Although the adverse effects of arsenic (As) are a matter of great concern, exposure to this notorious metalloid is inevitable. In order to develop an efficient, cheap, and eco-friendly adsorbent to remove As from water, molecular dynamic simulation using Material Studio 2017 software is performed to understand the behaviour of cellulose as an adsorbent. Modification of cellulose with different functional groups is studied, and calculations of adsorption energy and density functional theory (DFT) are performed. Various electronic properties like charge density, binding energy, radial distribution function, total energy, as well as energy convergence, have been calculated to find out the most efficient structure for adsorption of As. Amongst all the modifications, i.e., –SH, –COOH, CH3COO-, –NH2, cellulose functionalized with –SH shows an optimum result in terms of energy (highest occupied molecular orbital energy, 4.817 eV), surface area (470.29Å2) and surface volume (490.37Å3) which gives a strong inference of using cellulose material and its –SH modified structure as a suitable and potential biosorbent for As removal.

Table1:- HOMO, LUMO, Chemical potential (μ), Hardness (ղ), Electrophilicity (ω), Maximum electronic charge (ΔN), Global Softness (S), Electronegativity (ꭓ)

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| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Molecule | HOMO (eV) | LUMO (eV) | μ | ղ | ω | S | ΔN | ꭓ |
| Cellulose | -5.814 | 0.506 | -2.654 | 1.58 | 2.229 | 0.3164 | 1.679 | 2.65 |
| Aminocellulose | -5.043 | 0.58 | -2.2315 | 1.4057 | 1.7711 | 0.35568 | 1.5874 | 2.2315 |
| Thiocellulose | -4.817 | -0.934 | -2.875 | 0.97075 | 4.25882 | 0.515065 | 2.962142 | 2.8755 |
| Acetylocellulose | -5.988 | -1.174 | -3.581 | 1.2035 | 5.3276 | 0.415454 | 2.975488 | 3.581 |
| Carboxyl cellulose | -5.514 | -1.225 | -3.369 | 1.07225 | 5.9426 | 0.4663092 | 3.14245744 | 3.3695 |

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