

## Efficient removal of pharmaceuticals from water using graphene nanoplatelets as adsorbent

### ABSTRACT

Recently, pharmaceutical pollutants in water have emerged as a global concern as they give threat to human health and the environment. In this study, graphene nanoplatelets (GNPs) were used to efficiently remove antibiotics sulfamethoxazole (SMX) and analgesic acetaminophen (ACM) as pharmaceutical pollutants from water by an adsorption process. GNPs; C750, C300, M15 and M5 were characterized by high-resolution transmission electron microscopy, Raman spectroscopy, X-ray diffraction and Brunauer–Emmett–Teller. The effects of several parameters viz. solution pH, adsorbent amount, initial concentration and contact time were studied. The parameters were optimized by a batch adsorption process and the maximum removal efficiency for both pharmaceuticals was 99%. The adsorption kinetics and isotherms models were employed, and the experimental data were best analysed with pseudo-second kinetic and Langmuir isotherm with maximum adsorption capacity ( $Q_m$ ) of 210.08 mg g<sup>-1</sup> for SMX and 56.21 mg g<sup>-1</sup> for ACM. A regeneration study was applied using different eluents; 5% ethanol-deionized water 0.005 M NaOH and HCl. GNP C300 was able to remove most of both pollutants from environmental water samples. Molecular docking was used to simulate the adsorption mechanism of GNP C300 towards SMX and ACM with a free binding energy of -7.54 kcal mol<sup>-1</sup> and -5.29 kcal mol<sup>-1</sup>, respectively, which revealed adsorption occurred spontaneously.

**Keyword:** Pharmaceutical; Removal; Graphene; Sulfamethoxazole; Acetaminophen; Environmental samples