

2D materials functionalization under visible light irradiation

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Two-dimensional nanomaterials seems to be a perspective for creating new devices for a wide range of applications [1]. Instead of synthesis of new materials having exotic chemical compositions a promising alternative is the functionalization of the known structures, like transition metal dichalcogenides (TMDs) or graphene oxide (GO), to give them the desired properties [2,3]. By functionalizing the surface of two-dimensional nanomaterials, it is possible to significantly improve their characteristics and by selecting the appropriate functional groups and the type of adsorbed molecules, it is possible to create nanomaterials with the specified characteristics. The purpose of this work was to theoretically investigate the features of the atomic structures and physical properties of TMDs and GO monolayers functionalized by chemical groups and organic molecules. The effect of the functionalization of molecular groups on the electronic structure and optical properties of TMDs and GO was evaluated. The information obtained opens new prospects of the application of functionalized monolayers in optoelectronics devices. The work was supported by the Russian Science Foundation (No. 21-73-10238).

- [1] Zhang H, Chhowalla M and Liu Z 2018 *Chemical Society Reviews* **47** 3015–3017
- [2] Azadmanjiri J, Kumar P, Srivastava V K and Sofer Z 2020 *ACS Applied Nano Materials* **3** 3116–3143
- [3] Jones L O, Mosquera M A, Ratner M A and Schatz G C 2020 *ACS applied materials & interfaces* **12** 4607–4615