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Modelling 2D Nanoflake - Bacterium Interactions in Solutions

Abstract:

Understanding the interaction between nanomaterials and biological membranes is crucial for advancing applications in nanomedicine and antimicrobial therapies. Nanomaterials such as MoS_2 and WS_2 nanoflakes exhibit unique physical properties that could be used for biomedical applications. This study aims to investigate the interaction dynamics between a bacterium such as Staphylococcus aureus (S. aureus), potentially responsible for some important pathologies such serious forms of pneumonia, and two-dimensional (2D) nanoflakes of MoS_2 and WS_2. The model, based on Molecular Dynamics (MD) simulations, takes into account the material type, its affinity with the bacterial culture, and the concentration of the nanoflakes relative to the bacteria in solution. The study shows that nanoflake material and concentration significantly influence the interactions with and the dynamical approach to the bacterial surface, with MoS_2 and WS_2 displaying distinct behaviours. These insights help potential advance in the use of nanomaterials as antimicrobial agents.

Keywords: Staphylococcus aureus, Molecular Dynamics (MD) Simulations, Nanoflakes, Transition Metal Dichalcogenides (TMDs), Nanomaterials-Bacteria Interaction, LAMMPS

Department

University of Naples Federico II

Primary author(s) : LETO, Nicolas; Dr. ADAM, Jaber; Dr. CHIARIELLO, Andrea Maria (Dipartimento di Fisica Ettore Pancini, Università di Napoli Federico II); Dr. SINGH, Manjot; Dr. VALADAN, Mohammadhassan; Prof. DEL SORBO, Mariarosaria; Dr. BIANCO, Simona; ALTUCCI, CARLO (Dept. of Advanced Biomedical Sciences - Università degli Studi di Napoli Federico II); NICODEMI, MARIO (Università di Napoli "Federico II")

Presenter(s) : LETO, Nicolas; Dr. ADAM, Jaber