Surface interaction studies of novel 2D materials with gram-negative and gram-positive pathogens.

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Abstract

The interaction between 2D-nanoflakes and bacteria in water based physiological liquids is a hot topic in biosciences. In this work we extend the DLVO theory, to the case of 2D-nanoflakes interacting with bacteria cell membranes, both for gram-positive and gram-negative bacteria. We study the role of the bacterial shape, membrane potential and 2D-materials nature. We calculate the interaction distances at equilibrium for different bacterial species and MoS_2 nanomaterials in Water and Cyrene.

Introduction

The interaction of bacteria and nanoparticles[1] and with 2D-nanomaterials[2] are well studied. But still, there is more investigation needed—for example, studies of the interaction of different bacteria and different solvents. Here, we used DLVO **(Derjaguin-Landau-Verwey-Overbeek)**[3] model to understand how different types of **bacteria** (Three **Gram-positive** and **Three Gram-negative**), interact with **2D-nanomaterials (**MoS_2**)** in two different solvents **(Water and Cyrene)**, by studying surface **interaction energy**, and, how different characteristics of bacteria (such as ζ**-potential and radius**) affect their interaction energy.

Methodology

- **DLVO model** below equations (two main interactions, the attractive **van der Waals** $((V^{VW})$ and the repulsive **electrostatic** (V^{EL})**)** equation below.
- Six bacteria strains (**S.carnosus, S.maltophilia, N.subflava, B.subtilis, S.aureus and E.coli).**
- MoS_2 nanoflake in two different green solvents (**Cyrene and Water).**
- The **critical volume** r^3_{crit} (The critical volume around the bacteria where the attraction forces dominate)[1] is **calculated** by using below equation.

$$V^{tot} = V^{EL} + V^{VW}$$

$$V^{EL} = \frac{\pi\epsilon a_1 a_2(\zeta_1^2+\zeta_1^2)}{(a_1+a_2)}\left\{\frac{2\zeta_1\zeta_2}{\zeta_1^2+\zeta_1^2}\ln\left[\frac{1+exp(-kd)}{1-exp(-kd)}\right]+\ln[1-exp(-2kd)]\right\}$$

$$V^{VW} = -Aa_1a_2/6d(a_1+a_2)$$

$$r^3_{crit} = (d_{max}+a_1)^3 - a_1^3$$

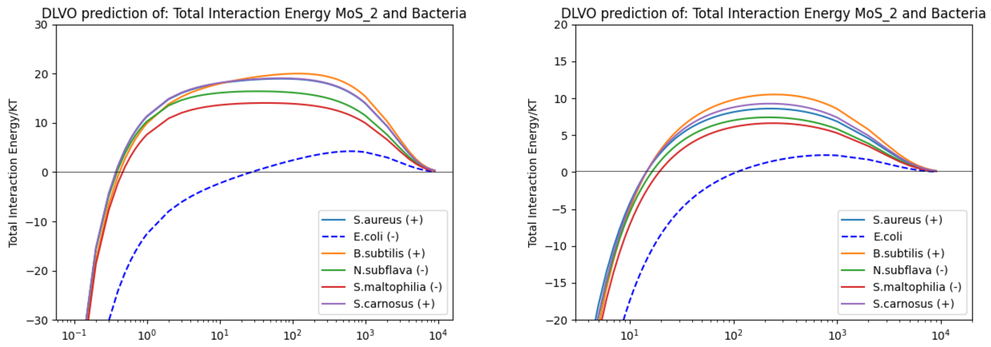

Figure 1: Total Interaction Energy of bacteria-MoS_2 for a) Water b) Cyrene.

	ζ-poten (mV)	a_1 (nm)	d_{water} (nm)	d_{cyrene} nm	V^{tot}_{water}/KT	V^{tot}_{cyrene}/KT	$r^3_{crit_w}$
B.subtilis (G+)	-41.00	520	120.00	249.98	20.00	10.51	12.20
S.carnosus (G+)	-37.00	440	68.00	224.98	19.05	09.27	04.50
S.aureus (G+)	-37.10	360	69.00	224.98	18.96	08.59	03.23
N.subflava (G-)	-30.00	400	33.00	217.98	16.41	07.41	01.72
S.maltophilia (G-)	-26.00	460	43.00	240.98	14.03	06.62	02.99
E.coli (G-)	-12.70	630	629.00	771.98	04.23	02.30	175.0

Table 1: Summary of different bacteria results and characteristic.

Results and Discussion

- The relation between **the total interaction energy** and **spacing** (d nm) between the **bacteria** and MoS_2 nanoflake for both **Water and Cyrene** Figure 1.
- **Higher** interaction of bacteria with **Water-based** solvent than that of **Cyrene** Figure 2 (a), mainly due to Water higher Hamaker constant.
- The **G+ bacteria** have **higher interaction energy** than **G-** due to the shape of bacteria and different ζ**-potential** (higher in the case of G+)Figure 1.
- Direct **proportionality** between the **interaction energy** and ζ**-potential** for both bacteria type.
- This pattern of results is consistent with the previous literature[1].
- **The radius** in the **G+** bacteria is **directly** proportional to **energy**, While the **radius** in the **G-** bacteria is **inversely** proportional to the **energy**.
- In Figure 2 (b) we selected **a single value for the spacing (**d**)**, plotted and compared the V^{vw} and V^{EL} for each solvent.
- The V^{EL} term is **dominant** for **Water** and V^{vw} **dominant** for the case of **Cyrene** Figure 2(b).

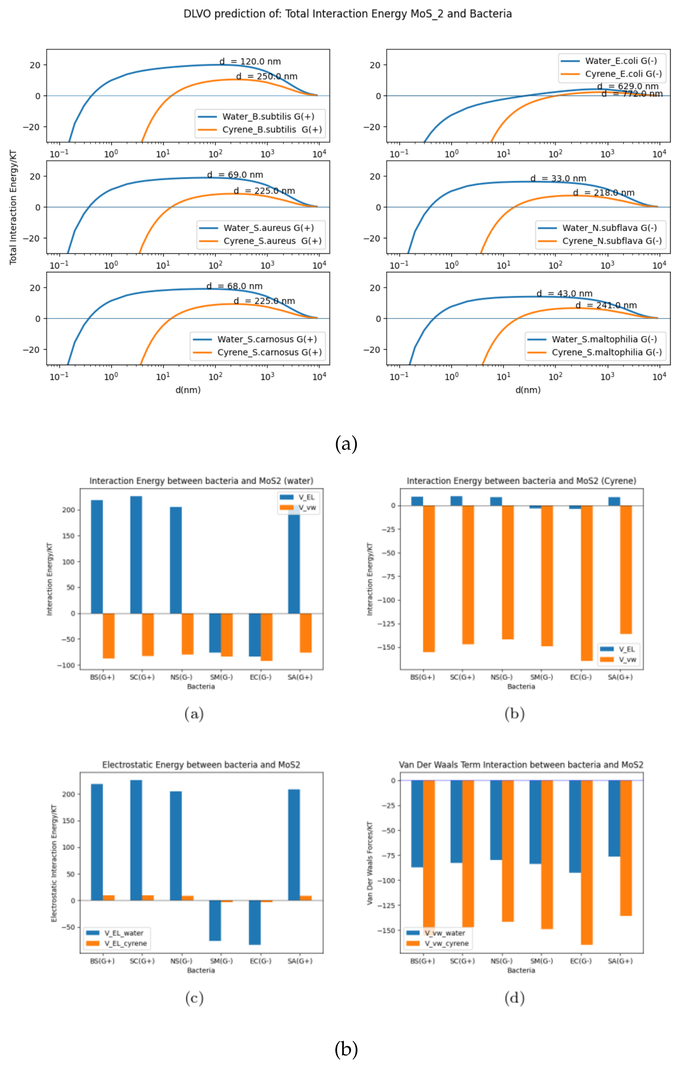

Figure 2: a) Comparison between Water and Cyrene based solvents MoS_2-bacteria Total Interaction Energy b) V^{EL} and V^{vw} Interaction for Water and Cyrene (Upper panel), V^{EL} and V^{vw} for each solvents. (lower panel)

Conclusion/prospectives

We examined the surface interaction of **bacteria** and MoS_2 **2D-nanoflakes** based on **two solvents** using **DLVO model**. We found that G+ bacteria have **higher interaction energy** than G- bacteria. Water-based solvent MoS_2 nanoflake **interacts more** than Cyrene. We found that as the negative value of ζ-potential **increase**, interaction energy **increase** as well. And the critical volume, as well as Electrostatic and Van der Waals, was calculated. Also, in terms of **future research**, it would be helpful to extend the present findings by examining others solvents and other 2D-nanomaterials.

References