Electronic Supplementary Material (ESI) for Nanoscale Advances.


Electronic Supplementary Information

# Ultrasensitive two-dimensional material-based MCF-7 cancer cell sensor driven by perturbation processes

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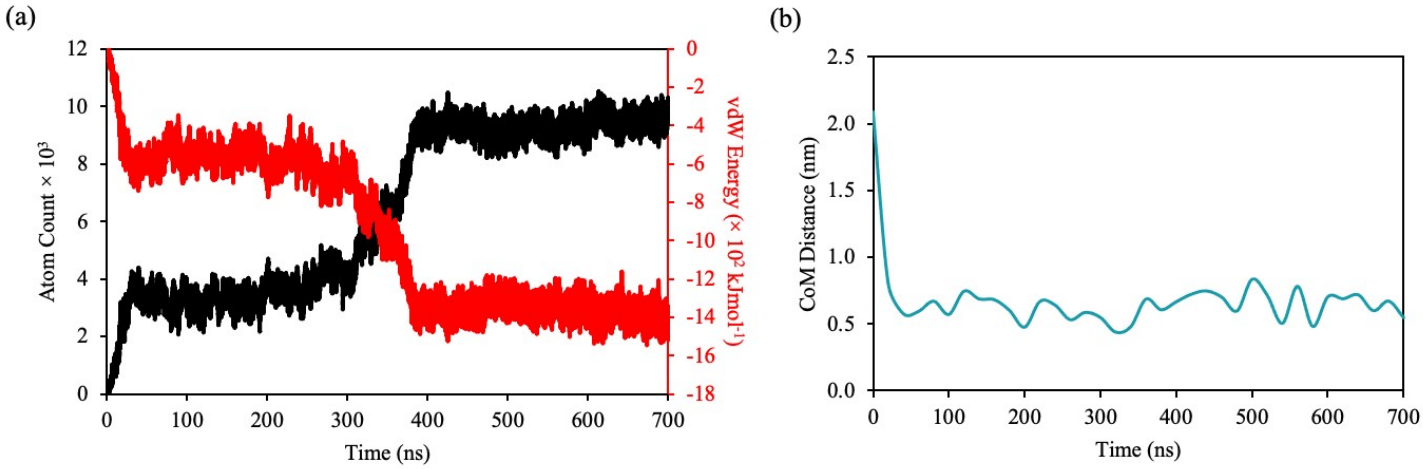


**Figure S1.** Computational analysis of $MoS_2$ and cancer lipid bilayer system. (a) Plot of atom count (black) and van der Waal (vdW) interaction energy (red, $kJmol^{-1}$) and (b) center of mass (CoM) distance (nm) plotted as a function of time (ns) for the interaction between $MoS_2$ nanosheet and cancer lipid bilayer system.

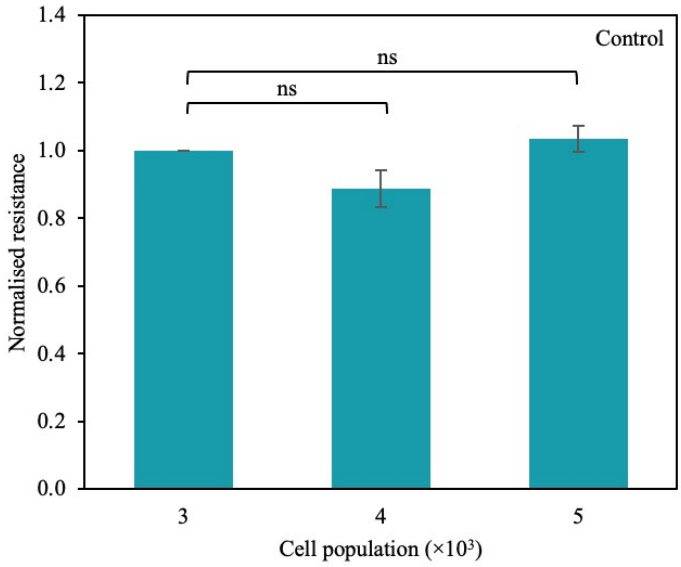


**Figure S2.** Normalised resistance for control (cells only, $3 \times 10^3$ cells) and MCF-7 cells at varying cell populations ($n = 4 \times 10^3$ cells and $5 \times 10^3$ cells). Data represents mean ± SEM, ($n = 6$ from 3 independent experiments). Significance was calculated using a Student's t-test: non-significant (ns).

**Figure S3.** Normalised resistance for MCF-7 media only and MCF-7 media with 75 μM of $MoS_2$ (Media/MS). Data represents mean ± SEM, ($n$ = 3). Significance was calculated using a Student's t-test: $p < 0.05$ (*)

**Table S1** Significance for MCF-7 cytotoxicity for different concentrations of $MoS_2$ compared to control, different concentrations of $MoS_2$ and different incubation times. Significance was calculated using a Student's t-test: $p < 0.05$ (*), $p < 0.01$ (**), $p < 0.001$ (***).

| | | Concentrations (μM) | | | |
|---|---|---|---|---|---|
| | | **25** | **50** | **75** | **100** |
| **MCF-7 (*t* = 24 h)** | Compared to Control | | | * | *** |
| | Compared to 25 μM | | | * | ** |
| | Compared to 50 μM | | | | ** |
| | Compared to 75 μM | | | | * |
| **MCF-7 (*t* = 48 h)** | Compared to *t* = 24 h | | | | |
| | Compared to Control | | | | * |
| | Compared to 25 μM | | | | |
| | Compared to 50 μM | | | | * |
| | Compared to 75 μM | | | | * |

**Table S2** Force field parameters for $MoS_2$,[1] where $\sigma$ is the finite distance (where interparticle potential is zero), $\varepsilon$ is the Lennard-Jones parameter referring to the depth of the potential well and *e* is the partial atomic charge.

| **Atom** | **σ /Å** | **ε /kJmol$^{-1}$** | ***e*** |
|---|---|---|---|
| Mo | 2.55 | 0.543 | -0.76 |
| S | 3.50 | 1.045 | -0.38 |

**Table S3** Lipid composition for the inner and outer leaflet of cancer lipid bilayer systems based on lipids built by Klähn & Zacharias.[2]

| | **Inner Leaflet** | | **Outer Leaflet** | |
|---|---|---|---|---|
| | DOPC | DOPS | DOPC | DOPS |
| **Cancer** | 91 | 30 | 99 | 22 |

**Table S4** Full references for Fig. 3d. State-of-the-art electrical-based biosensors detecting an adherent monolayer of cells.

| Ref No. | Reference |
|---|---|
| 1 | Yea, C. H., Jeong, H. C., Moon, S. H., Lee, M. O., Kim, K. J., Choi, J. W., Cha, H. J., In situ label-free quantification of human pluripotent stem cells with electrochemical potential. *Biomaterials* **75**, 250–259 (2016). |
| 2 | Jeong, H. C., Choo, S. S., Kim, K. T., Hong, K. S., Moon, S. H., Cha, H.. J., Kim, T. H., Conductive hybrid matrigel layer to enhance electrochemical signals of human embryonic stem cells. *Sensors Actuators, B Chem.* **242**, 224–230 (2017). |
| 3 | Suhito, I. R., Kang, W. S., Kim, D. S., Baek, S., Park, S. J., Moon, S. H., Luo, Z., Lee, D., Min, J., Kim, T. H., High density gold nanostructure composites for precise electrochemical detection of human embryonic stem cells in cell mixture. *Colloids Surfaces B Biointerfaces* **180**, 384–392 (2019). |
| 4 | Angeline, N., Choo, S. S., Kim, C. H., Bhang, S. H. & Kim, T. H. Precise Electrical Detection of Curcumin Cytotoxicity in Human Liver Cancer Cells. *Biochip J.* **15**, 52–60 (2021). |

## References


1 B. Luan and R. Zhou, *Appl. Phys. Lett.*, , DOI:10.1063/1.4944840.

2 M. Klähn and M. Zacharias, *Phys. Chem. Chem. Phys.*, 2013, **15**, 14427–14441.