Supporting Information for

Molecular Mechanism of Robust Macrophage Immune Responses Induced by PEGylated Molybdenum Disulfide

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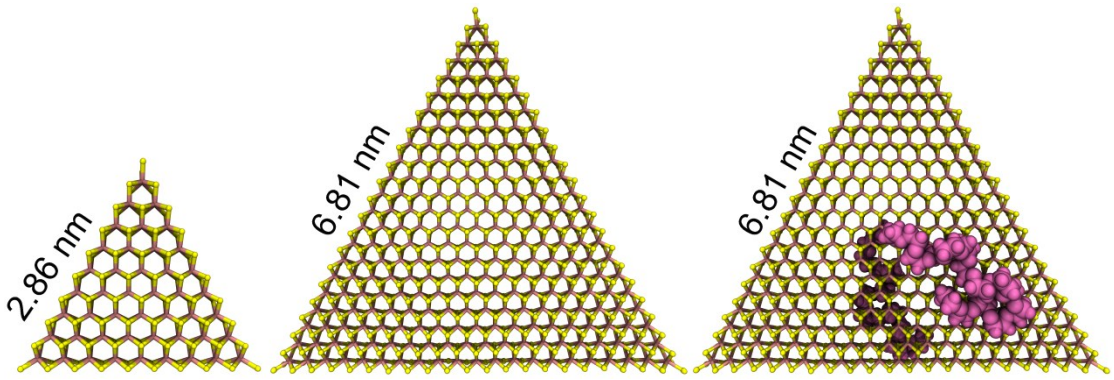

Figure S1. The MoS_2/MoS_2-PEG nanoflakes used in this study. MoS_2 is shown in a yellow and pink ball-and-stick representation. The two PEG chains are displayed in mauve spheres, one chain at each side of the MoS_2 basal plane.

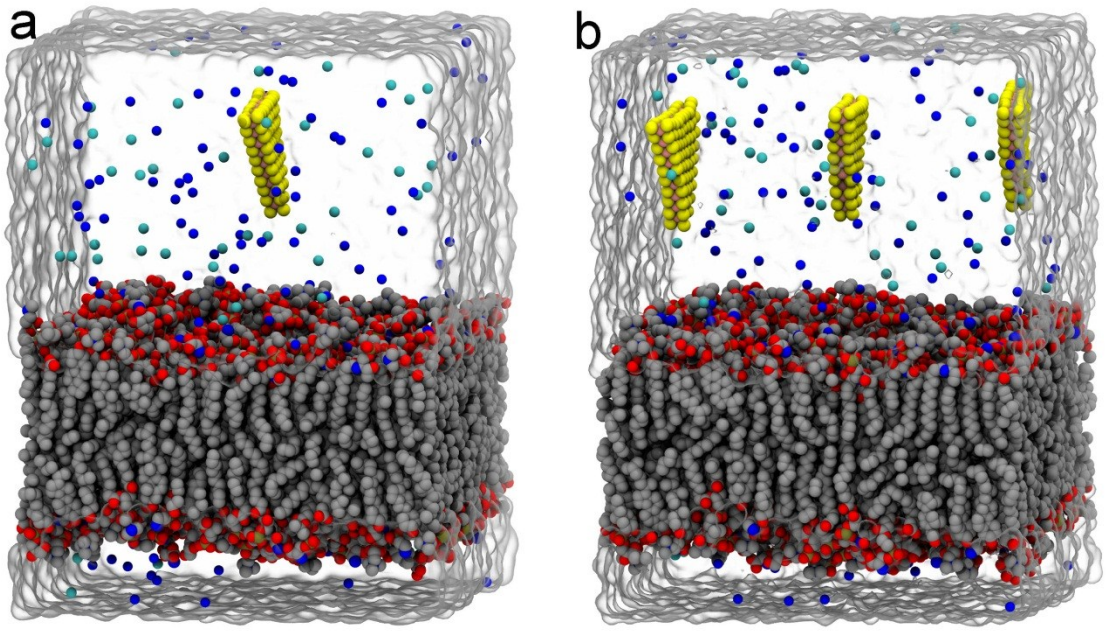

Figure S2. Initial simulation setups of the one and three small MoS_2 nanoflakes with the macrophage membrane. The lipid carbon atoms are represented in gray, oxygen atoms in red, nitrogen atoms in blue, and phosphorus atoms in purple, respectively. The MoS_2 sulfur atoms are rendered in yellow and molybdenum atoms in pink. The Na^+ and Cl^- ions are displayed in blue and cyan spheres, respectively. The water boundaries are indicated by white surfaces.

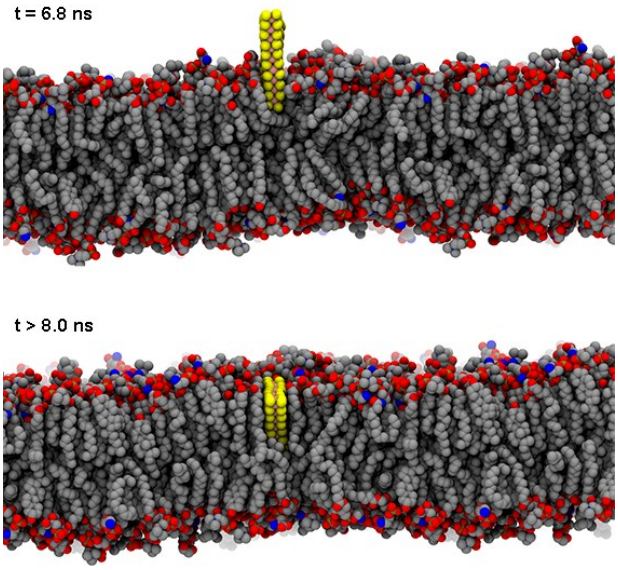

Figure S3. Snapshots from the molecular dynamics simulations of sys-1 at 400 K.

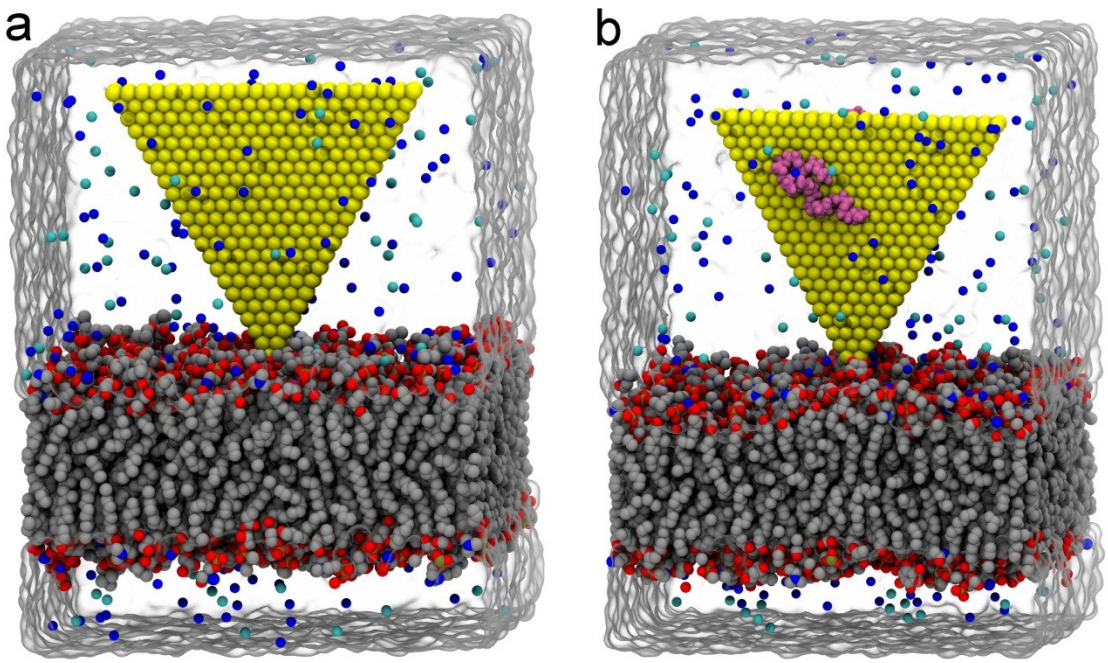

Figure S4. Initial simulation setups of the macrophage membrane with the large MoS_2 and MoS_2-PEG nanoflakes placed in corner point-on configurations.

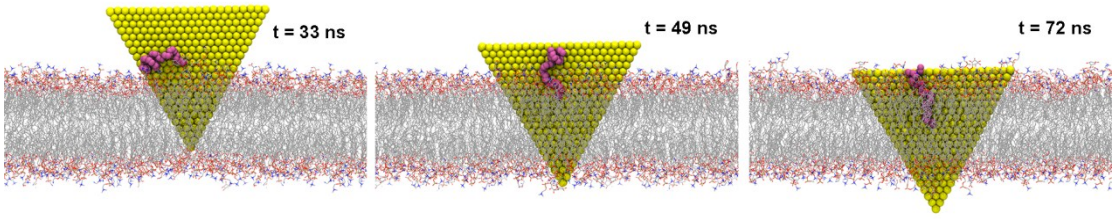

Figure S5. The orientation of PEG relative to the membrane during the insertion process.

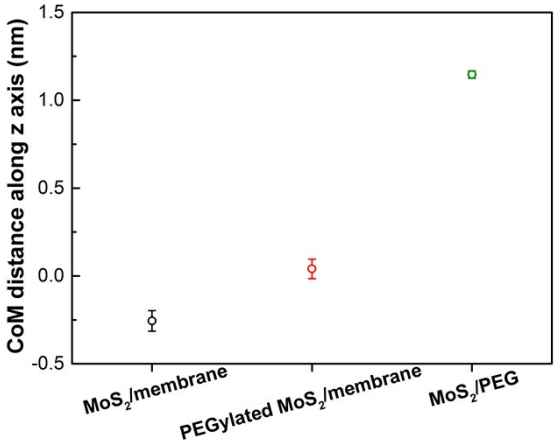

Figure S6. Averaged center of mass (CoM) distances between the macrophage membrane and

MoS_2/MoS_2-PEG or between MoS_2 and PEG in three parallel simulations of sys-3 and sys-4.

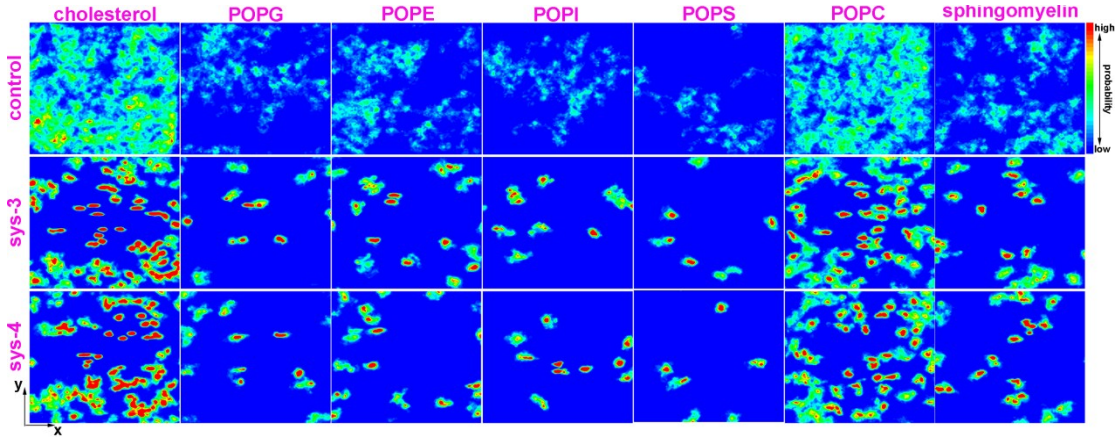

Figure S7. 2D x-y distribution probabilities of each lipid type in outer leaflet.

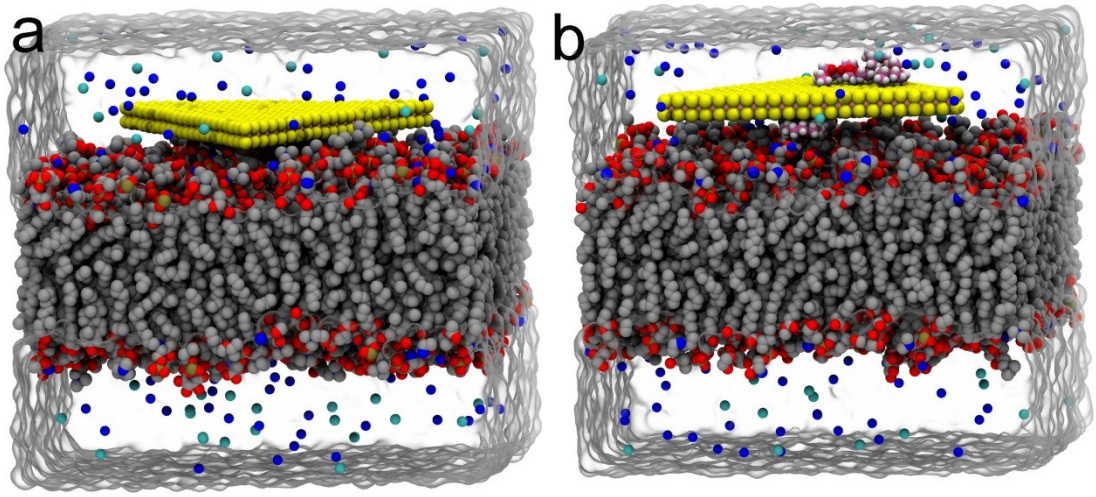

Figure S8. Initial simulation setups of the macrophage membrane with the large MoS_2 and MoS_2-PEG nanoflakes placed in face-on configurations.

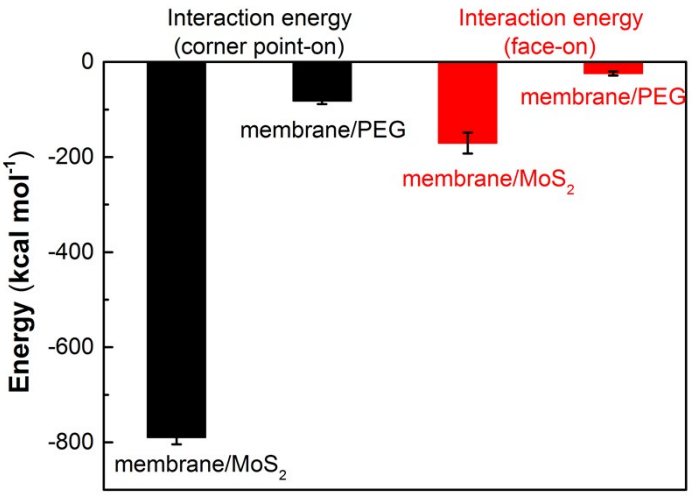

Figure S9. Decomposed interaction energies in corner point-on and face-on configurations. The energies were averaged from last 10 ns in each trajectory.

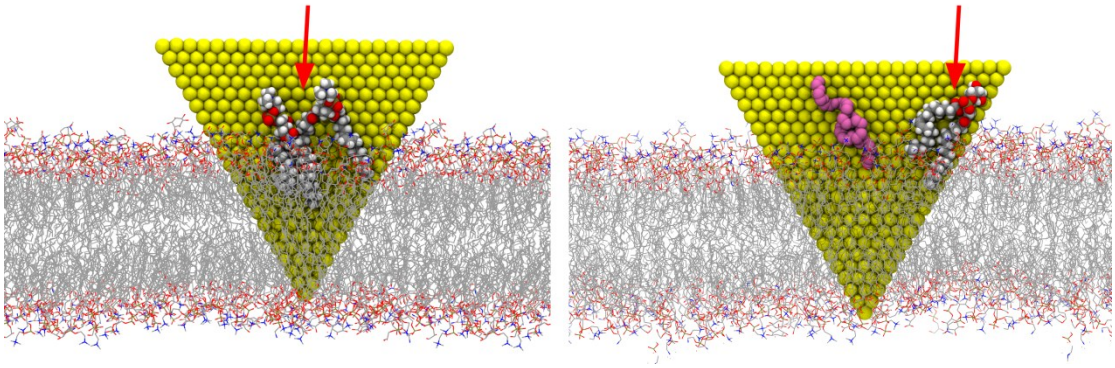

Figure S10. Lipid extraction by MoS_2 and MoS_2-PEG. The extracted lipids are shown in spheres and indicated by red arrows, while the other lipids are depicted in lines.

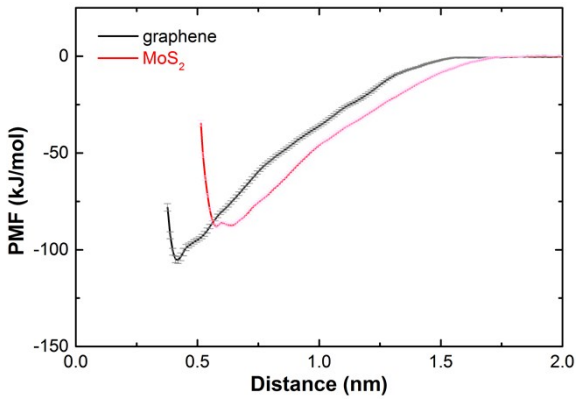

Figure S11. PMF of a POPC molecule binding to graphene and MoS_2 surface. The x-axis indicates the center of mass (CoM) distance between graphene/MoS_2 and POPC.

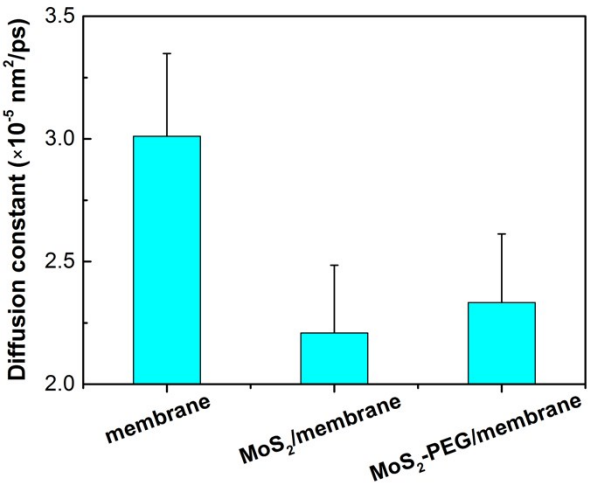

Figure S12. Membrane diffusion constants of the MoS_2/membrane and MoS_2-PEG/membrane systems. The diffusion constant was computed based on the head group atoms in the outer leaflet of the membrane. The trajectories from face-on configurations were used for the calculations.

Table S1. Simulation system details.

	Box size (nm^3)	**Number of water molecules**	**Simulation time (ns)**
sys-1 (one small MoS_2)	10.00×10.00×12.51	26,232	300
sys-2 (three small MoS_2)	10.00×10.00×12.50	26,022	300
sys-3 (one large MoS_2, corner point-on)	10.00×10.00×13.93	30,881	150
sys-4 (one large MoS_2-PEG, corner point-on)	10.00×10.00×13.91	30,548	150
sys-5 (one large MoS_2, face-on)	10.00×10.00×9.59	20,401	1000
sys-6 (one large MoS_2-PEG, face-on)	10.00×10.00×9.47	20,372	1000