



- Umbrella sampling technique
- The new FF was used to predict adsorption free energies of 20 naturally-occurring amino acids at the aqueous MoS₂ interface.
- This library can be used to design peptides for MoS₂ surface applications

Peptides sequences experimentally identified to have strong and weak binding affinity to the MoS₂ surface

Peptide	Sequence	Affinity	Ref.
MoSBP1	<u>Y</u> SATFT <u>Y</u>	Strong	57
HLL	HLLQPTQN <u>P</u> FRN	Strong	58
MoS2-P15	GVIH <u>R</u> NDQ <u>W</u> TAPGGG	Strong	22
MoS2-P28	<u>D</u> <u>R</u> <u>W</u> V <u>A</u> RD <u>P</u> ASIFGGG	Strong	22
MoS2-P3	SVMNTSTKDAIEGGG	Weak	22
MoSBP20	TSHMSNT	Weak	57