

Abstract Submitted  
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**Selective nesting and sensing of molecules on optimally modified material surfaces** JOHN RUSSELL, BOYANG WANG, PETR KRAL, University of Illinois at Chicago, PROF. KRAL'S RESEARCH GROUP TEAM — We develop a methodology of optimal modifications of material surfaces allowing us to design selective nesting sites for inorganic, organic and biological molecules [1]. The idea is to modify material surfaces by atomic dopants and charged ligands in such a way that the created local electric fields form selective Coulombic traps for the adsorbed molecules. We demonstrate this methodology by molecular dynamics simulations of short peptides docked in nesting sites designed on graphene sheets substitutionally doped with B and N atoms. We show that the same approach can be used to selectively dock proteins in water solvent on graphene layers modified by short charged ligands. As a practical application of this methodology, we design and model chemical sensors that could detect the selectively nested molecules. The detection is realized by evaluating the change of the electrical conductivity of the modified graphene sheets upon the docking of the molecules. [1] B. Wang and P. Kral, *Small*, 3, 580, (2007). [2] J. Russell, B. Wang and P. Kral, in preparation.

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