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Highly Sensitive Molecular Sensing on Optimally Modified Graphene Monolayers JOHN RUSSELL, PETR KRAL, University of Illinois at Chicago — We develop a methodology of molecular sensing on optimally modified graphene monolayers. The idea is to modify the monolayers by atomistic (substitution) doping or by covalent binding of short charged ligands at selected positions in such a way that the created local electric fields form selective molecular nests for inorganic, organic and biological molecules [1]. We show by molecular dynamics simulations the nesting of small organic molecules and peptides on modified graphene ribbons. The nested molecules can be detected by electronic, optical or vibrational means [2]. The method is highly sensitive and, at low temperatures, it can even distinguish the configurations of the nested molecules.

[1] B. Wang and P. Král, Small 3, 580 (2007).

[2] J. Russell and P. Král, in preparation.

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