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Molecular Bound States of Supercritical Charged Impurities on Graphene¹ KIRILL VELIZHANIN, LYUDMYLA ADAMSKA, Los Alamos National Laboratory, DMITRY SOLENOV, Saint Louis University — Functionalization of graphene by chemical groups/atoms allows one to tune its electronic, chemical and mechanical properties. For example, metallic adatoms (e.g., Li, Ca, Y) can be important in applications ranging from hydrogen storage to superconductivity. Such adatoms bind ionically to graphene and the resulting positive ions move along graphene relatively freely, so understanding the energetics of their interaction with graphene and between each other becomes critical for assessing stability of resulting materials in practical applications. It has recently been demonstrated that ions with charge greater than $Z \sim 1$ induce a very peculiar non-linear electronic polarization of graphene, which is reminiscent to the Dirac vacuum reconstruction around superheavy nuclei. In our work we demonstrate that such non-linear polarization qualitatively changes not only graphene electronic structure but also the energetics of the effective graphene-mediated interaction between such ions. In my talk, I will discuss the properties of such effective interaction and its dependence on various parameters of the system. In particular, I will report on our finding that molecular bound states of supercritically charged ions can be formed on graphene at certain conditions.

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