The issues and the theoretical strategies to deal with charged defects on periodic systems.

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Abstract: an increasing demand for new optical/electronic materials has been requested by the consumer market of new technologies. Thus, the study of semiconductor materials and their defects catch a great attention in several scientific areas. Charged defect systems play an important role on this scenario and the treatment of these systems presents some peculiarities on the periodic simulation approaches. On this seminar, it will be presented the mathematical and the physical specificities of the treatment of charged defects by the *ab initio* periodic methods. The corrective methods like *Hartree Coulomb cutoff*, *point counter charge* and *density counter charge* will be briefly presented. As well as, a new approach to correct the electrostatic interactions of periodic and quasi-periodic charged system will be discussed and compared to some reference calculations. To elucidate the issues and the progresses on charged defects calculations, the profile of the formation energy of positive defects on the ionic slab systems NaCl, NaF, LiF and MgO will be reported and discussed as well.