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Electric field polarization calculations using charge patching method[1] LIN-WANG WANG, Lawrence Berkeley National Lab, Berkeley CA 94720, XAVIER CARTOIXA SOLER, Universidad Autonoma de Barcelona, Barcelona, SPAIN — Charge patching method has been used to calculate the electronic structures of thousand atom nanosystems with ab initio accuracy. Within the charge patching method, the ab initio charge density of a nanostructure is patched together using charge motifs which are calculated from small prototype systems. However, the current charge patching method can only be used for systems without long range electric field. In this talk, we will present results which include the polarizations of charge motifs. These polarization motifs accurately describe the charge responses of a nanosystem under external electric fields, and the results agree well with direct ab initio calculations, including part of the local field effects. This motif polarization method enables us to calculate nanosystems such as charged impurities, quantum dots with permanent dipole moments, or charged quantum dots. It also makes it possible to calculate the charge density of a nanosystem selfconsistently when combined with the folded spectrum method in solving a few band edge electronic states.

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