Electrostatics in Periodic-boundary Conditions and Real-space Corrections ISMAILA DABO, NICOLA MARZARI, Massachusetts Institute of Technology — We address periodic-image errors arising from the use of periodic-boundary conditions to describe systems that do not exhibit full three-dimensional periodicity. We show that the difference between the Coulomb potential calculated by Fourier transforms and the exact potential can be characterized analytically. Based on this observation, we present an efficient real-space method to correct periodic-image errors in plane-wave calculations. Comparing the method with existing schemes, we show that it is particularly advantageous for studying systems exhibiting one- or two-dimensional periodicity. As an application, we consider the vibrational properties of CO adsorbed on charged platinum surfaces.