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Polarons in thin Ga_2O_3 layers[1] HARTWIN PEELAERS, University of California, Santa Barbara, JOEL B. VARLEY, Lawrence Livermore National Laboratory, CHRIS G. VAN DE WALLE, University of California, Santa Barbara — Ga_2O_3 has a large band gap of 4.9 eV, making it transparent in the UV. It can also be doped n-type, enabling applications as a transparent conductor or in power electronics. The optical properties of Ga_2O_3 may be affected by the formation of small polarons, i.e., localized holes trapped by a lattice distortion. First-principles calculations have established the stability of such polarons in bulk Ga_2O_3 [J. B. Varley *et al.*, Phys. Rev. B **85**, 081109(R) (2012)]. Here we investigate hole polarons in nanomembranes of Ga_2O_3. We perform first-principles calculations based on density functional theory using a hybrid functional. Since polarons correspond to positive charges, a neutralizing charge needs to be included in supercell calculations. The use of a jellium background leads to divergence problems in low-dimensional systems. To prevent this, we modified the charge of the pseudopotentials, thus providing charge compensation that is confined within the layer. Our results obtained with this technique show that small polarons can indeed be formed in thin layers. Comparisons with polarons in the bulk and with experiments will be discussed.

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