Contact charging between single-crystal oxides from first principles electronic structure calculations and experiments

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***Abstract*— First principles electronic structure calculations are carried out to predict contact charging between surfaces. The calculations are performed on single-crystal alumina (sapphire) and silicon oxide (quartz) surfaces which have well-ordered repeat units that make the high level calculations practical. To validate the calculations, contact charging experiments with the same surfaces are carried out in a humidity-controlled environment. Both experiments and calculations show that sapphire charges positively and quartz charges negatively, with a magnitude of 10 $\mu C/m^2$. These results indicate the possibility of quantitatively predicting and explaining contact electrification from only the atomistic structure of material surfaces.**