

Using DFT and post-DFT methods to predict the interaction of water with SrTiO₃

E. Holmström¹ and A. S. Foster^{1,2}

¹COMP, School of Science, Aalto University, P.O. Box 11100 FI-00076 AALTO, Finland

²Frontier Science Organization, Kanazawa University, Kanazawa, 920-1192, Japan

email: eero.holmstrom@aalto.fi

For the past two decades, the standard quantum-mechanical approach to modeling adsorption of molecules onto surfaces has been density functional theory (DFT). At the same time, it has become clear that the result of a standard DFT calculation of such an adsorption process is very sensitive to how the computation is set up, *i.e.*, the choice of exchange-correlation functional, dispersion correction, and other possible ingredients such as a Hubbard $+U$ correction for systems containing transition metals. Choosing the adsorption of water onto the prototypical metal-oxide photocatalyst SrTiO₃ as an example, we use semi-local DFT, hybrid-functional DFT, and the wavefunction-based MP2 method to break beyond the traditional DFT-based paradigm. Through our results, we seek an improved and accurate understanding of this intricate adsorption process. In addition, we assess the accuracy of semi-local and non-local DFT and established dispersion corrections to these in describing the water-metal-oxide interaction. Finally, we probe general implications of our results for the first-principles modeling of surface reactivity.