Layered transition metal oxides (LTMOs) can intercalate small ions into their structure, making them effective electrodes for batteries. There is therefore a strong technological interest on developing new generations of this class of compounds. Density functional theory (DFT) is helping in this quest; however, conventional DFT approaches have serious shortcomings to treat van der Waals (vdW) forces; vdW interactions are indeed a crucial structural ingredient to describe LTMOs. This casts a shadow over the descriptive capabilities of DFT when applied to these materials. Recent exciting developments in DFT allow us now to tackle this problem head on.

Here we employed vdW-inclusive methods based on nonlocal density functionals [1] to thoroughly explore the role of vdW forces in key thermodynamic and kinetic properties of alkali and alkaline-earth ion insertion into $V_2O_5$ [2]. We find that vdW forces stabilize inserted ions and, therefore, increase cell voltages compared to conventional density functionals. Moreover, ion diffusion energies significantly increase as a consequence of vdW interactions. These results highlight the relevance of vdW forces to ion intercalation and dynamics in LTMOs.