

SI for

## Liquid phase exfoliation of $\text{MoO}_2$ nanosheets for lithium ion battery applications

John B. Boland,<sup>1,2</sup> Andrew Harvey,<sup>1,2</sup> Ruiyuan Tian,<sup>1,2</sup> Damien Hanlon<sup>1,2</sup> Victor Vega-Mayoral,<sup>1,2</sup> Beata Szydłowska,<sup>1,2</sup> Aideen Griffin,<sup>1,2</sup> Tanja Stimpel-Lindner,<sup>3</sup> Sonia Jaskaniec,<sup>1,4</sup> Valeria Nicolosi,<sup>1,4</sup> Georg Düsberg<sup>3</sup> and Jonathan N. Coleman<sup>1,2\*</sup>

<sup>1</sup>CRANN & AMBER Research Centers, Trinity College Dublin, Dublin 2, Ireland

<sup>2</sup>School of Physics, Trinity College Dublin, Dublin 2, Ireland

<sup>3</sup>Universität der Bundeswehr München, Werner-Heisenberg-Weg 39, D-85577 Neubiberg, München, Deutschland.

[\\*colemaj@tcd.ie](mailto:colemaj@tcd.ie)

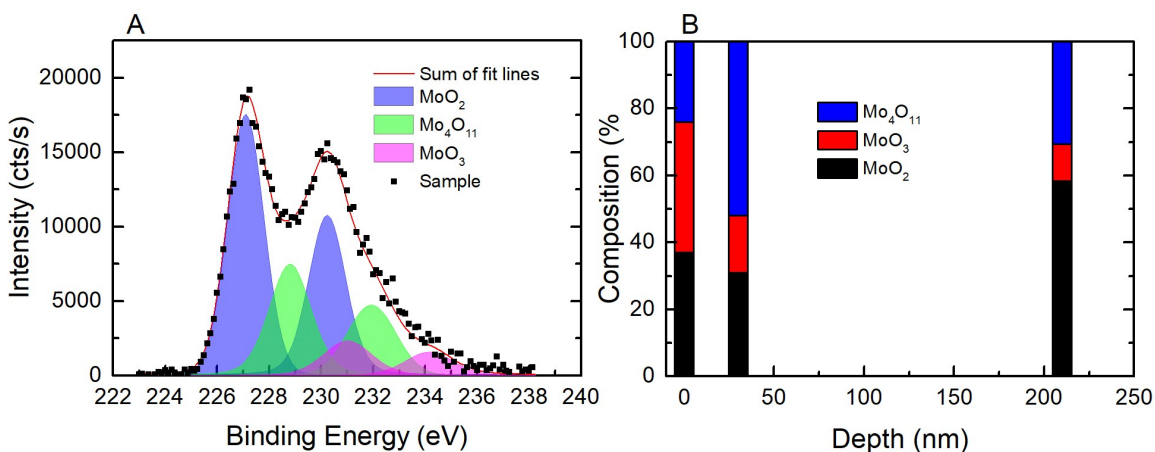


Figure 1: XPS analysis of  $\text{MoO}_2$  films made by vacuum filtration. A shows the measured XPS spectrum of the sample and its fitted components. The sum of these fits is also shown for comparison with the observed spectrum. B indicates the variance of composition with sputtering depth.

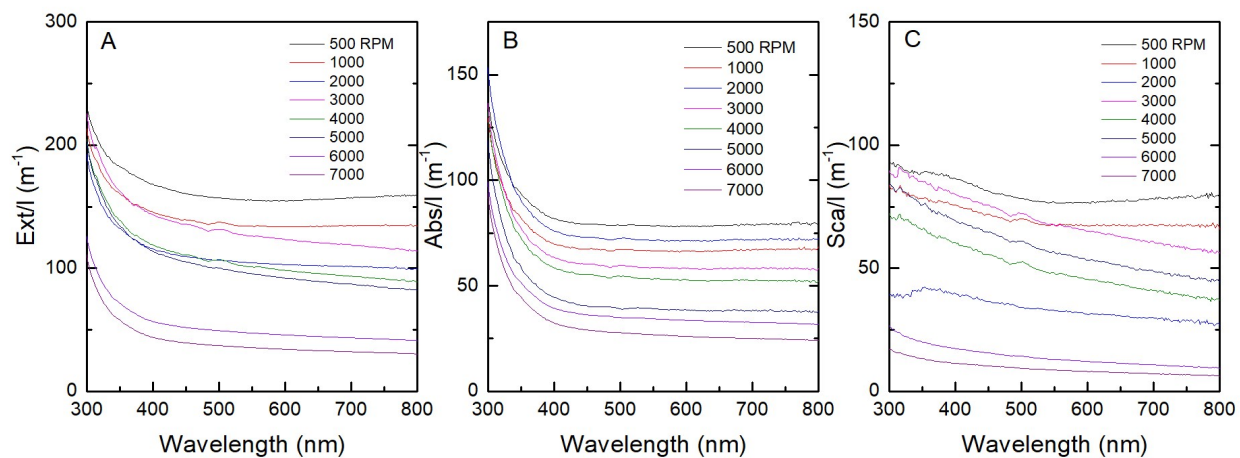


Figure 2: Centrifugation study of MoO<sub>2</sub> in CHP. A-C show the Extinction, Absorption and Scattering spectra respectively from UV-vis spectroscopic analysis.

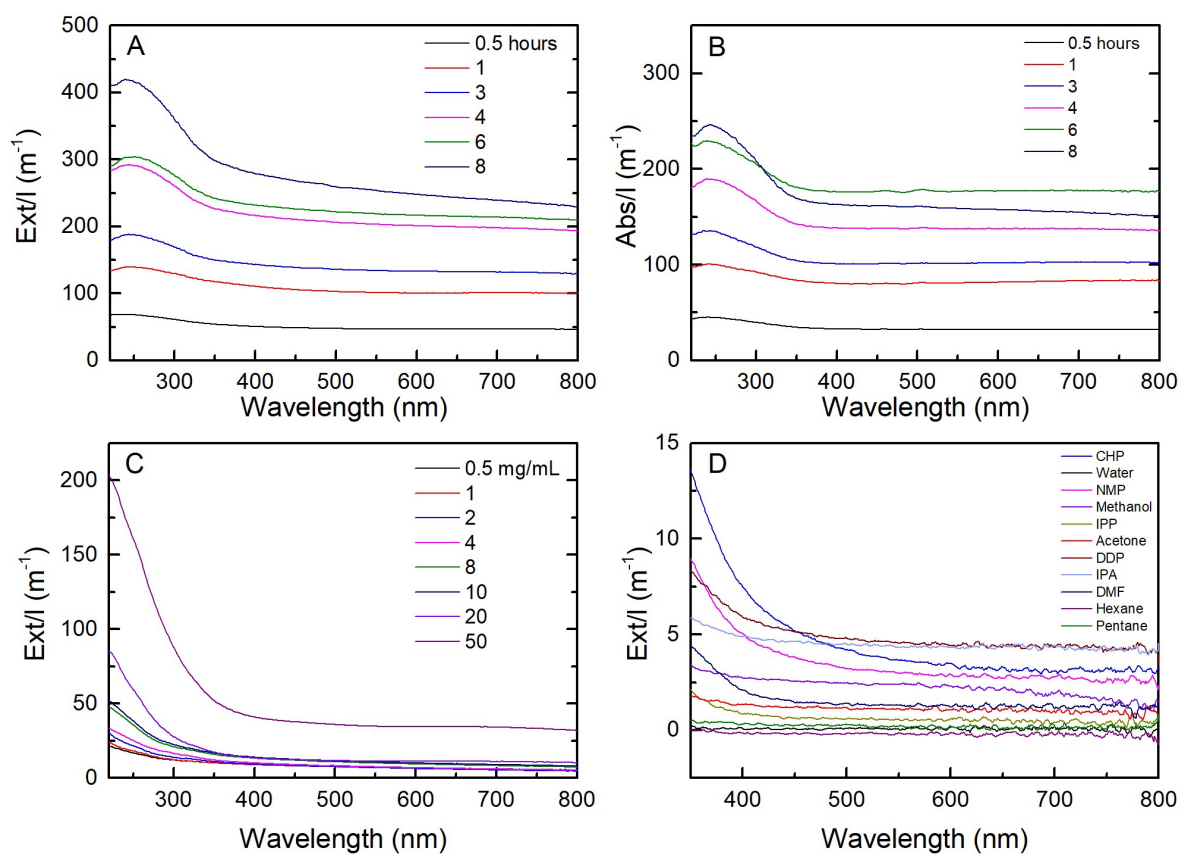


Figure 3: Optimization of the exfoliation process. A-B show UV vis spectra for a study on variation in sonication time, where A and B are the extinction and absorption respectively. C Initial concentration study, D Solvent study.

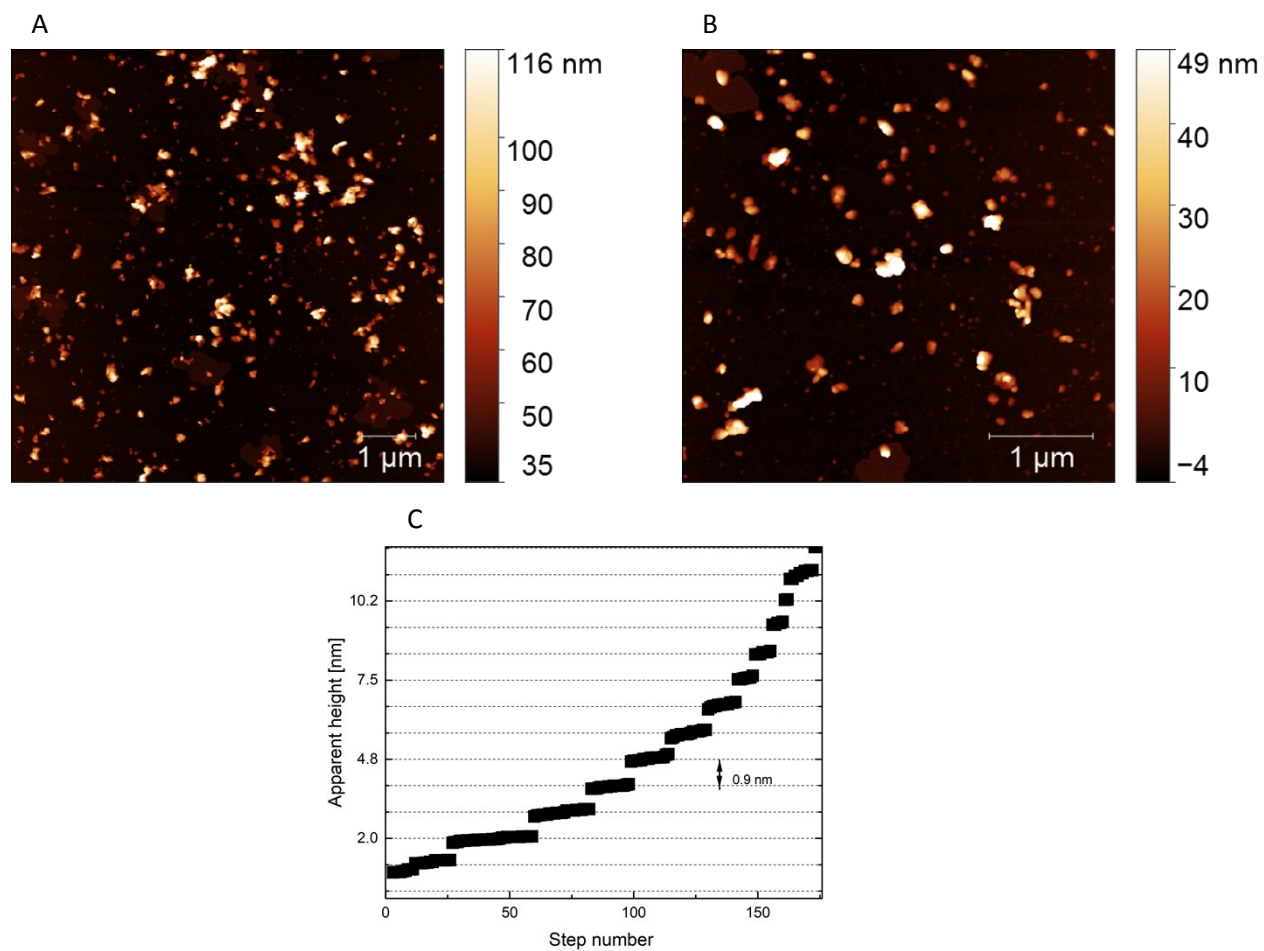


Figure 4: AFM analysis of  $\text{MoO}_2$  standard sample in IPA. A and B are representative AFM images. C is the step height analysis.

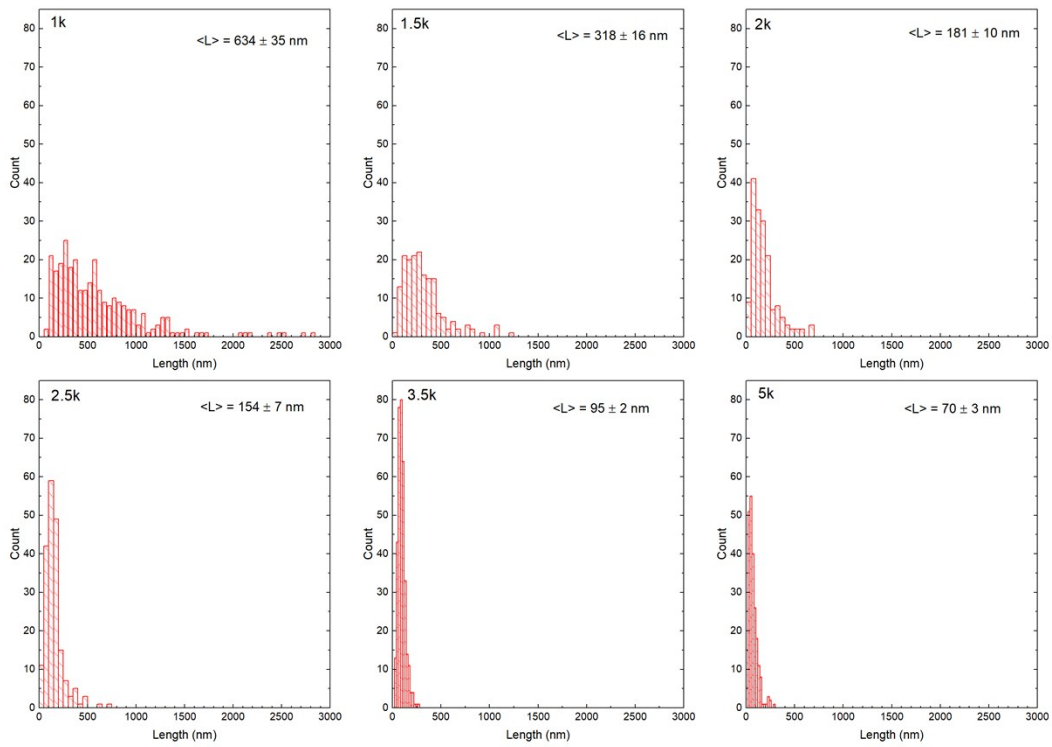


Figure 5: Flake size distribution of size selected samples from TEM analysis.

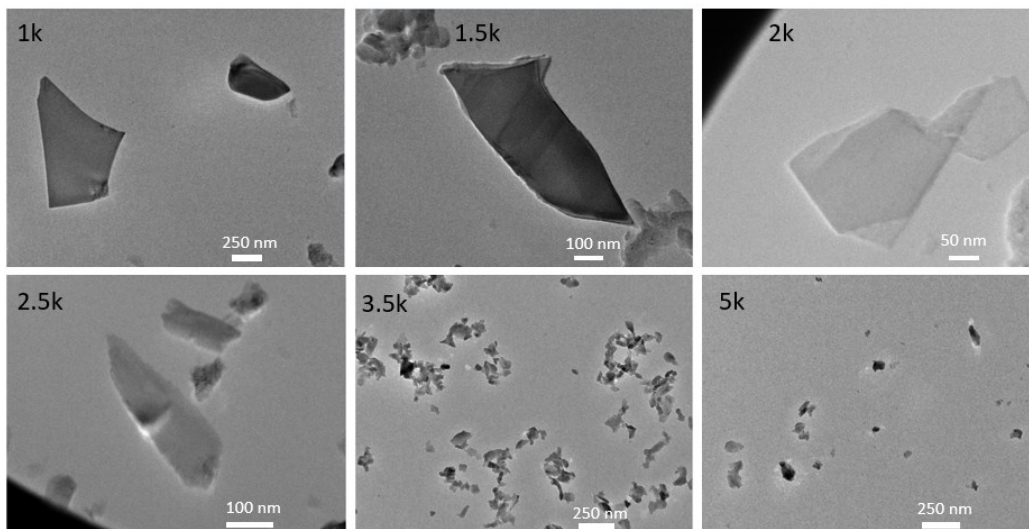


Figure 6: Representative TEM images from size selected samples.

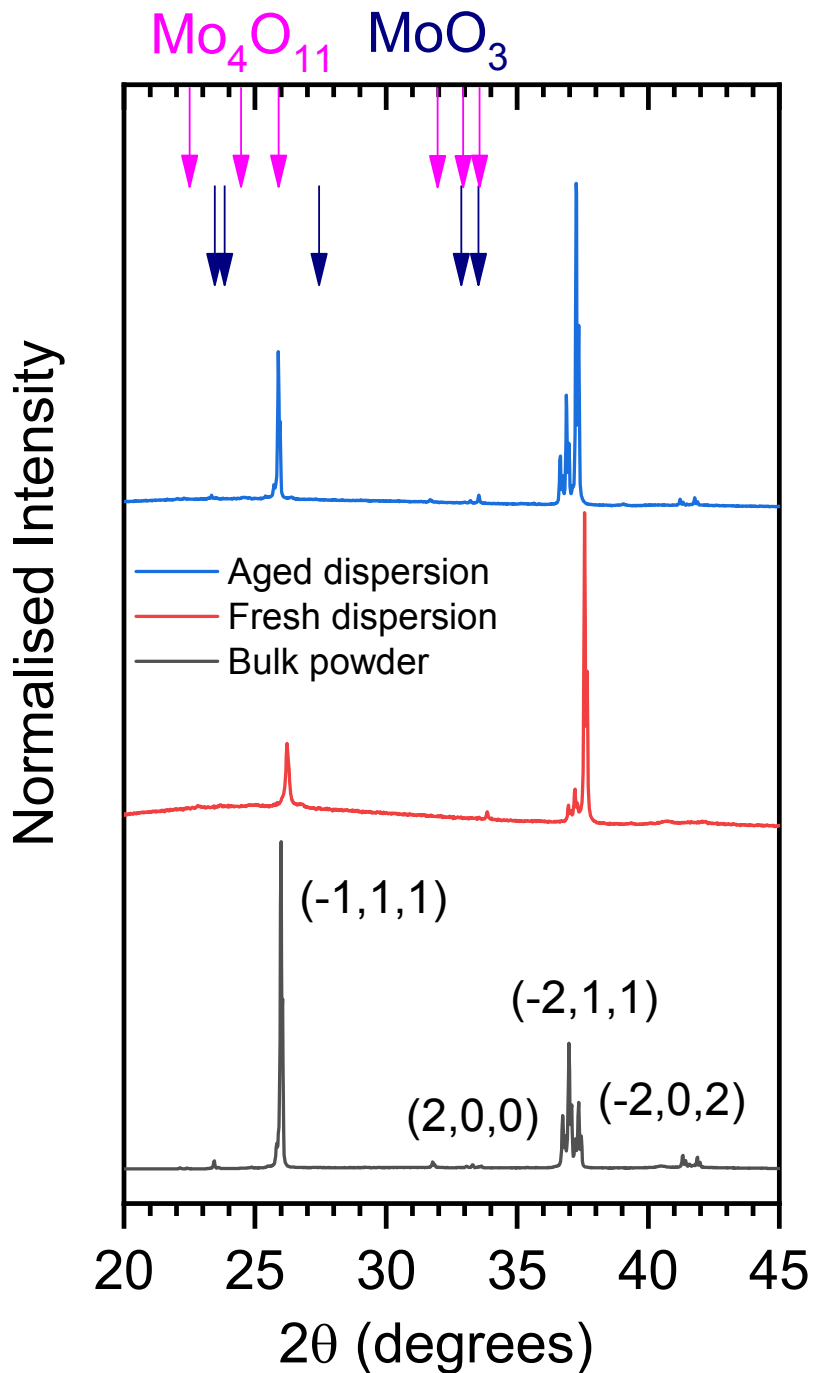


Figure 7: X-ray diffraction spectra for bulk  $\text{MoO}_2$  powder (black) as well as  $\text{MoO}_2$  nanosheets cast into a film from a fresh dispersion (red) and  $\text{MoO}_2$  nanosheets cast into a film from an aged dispersion (blue). The aged dispersion was stored in IPA for 2 months before testing. The magenta and navy arrows at the top represent the positions of the main lines for  $\text{Mo}_4\text{O}_{11}$  and  $\text{MoO}_3$  as reported by ref<sup>1</sup>.

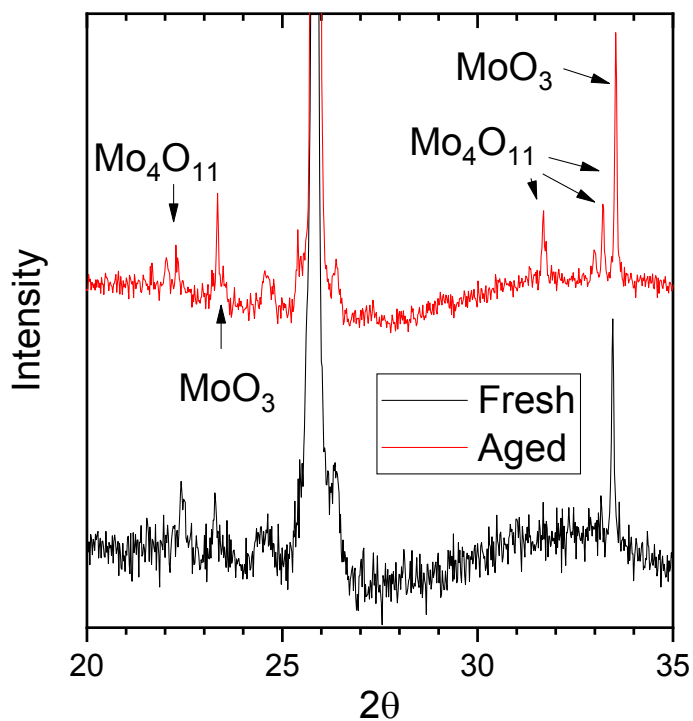


Figure 8: Comparison of weak peaks in fresh and aged nanosheet spectra. Weak MoO<sub>3</sub> and Mo<sub>4</sub>O<sub>11</sub> peaks can be seen, predominately in the aged sample.

X-Ray diffraction (XRD) measurements were performed in a Bruker Advance Powder X-Ray diffractometer equipped with Cu-K $\alpha$  emission source in Bragg-Brentano configuration. Bulk MoO<sub>2</sub> finely ground powder was directly deposited in a sample holder, while for the nanosheet dispersions, the measurements were done on thin films prepared on glass substrates.

1. T. Ressler, R. E. Jentoft, J. Wienold, M. M. Günter and O. Timpe, *The Journal of Physical Chemistry B*, 2000, **104**, 6360-6370.