On stability and kinetics of Li–rich transition metal oxides and oxyfluorides

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SUPPLEMENTARY INFORMATION

Structure of distorted Li₂VO₂F

FIG. 1: Structure of the distorted version of layered–like Li₂VO₂F, showing the coordination polyhedra (left) and projections along the a–axis (middle) and the c–axis (right). The slight shift of the V atoms is clearly visible in the projected structures.
Pair distribution function in DRS–type Li$_2$VO$_2$F and Li$_2$VO$_3$

FIG. 2: Pair distribution function of the DRS–type Li$_2$VO$_2$F and Li$_2$VO$_3$. The increased V–F distances in Li$_2$VO$_2$F and the resulting changes in the V distribution are clearly visible from comparison to the DRS oxide.
Di-vacancy diffusion pathways in Li$_2$VO$_2$F and Li$_2$VO$_3$.

FIG. 3: Di-vacancy diffusion: Diffusion pathways in the presence of di-vacancies for a) Li$_2$VO$_3$ and b) Li$_2$VO$_2$F (right).