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

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SUPPLEMENTARY INFORMATION

Structure of distorted Li_2VO_2F

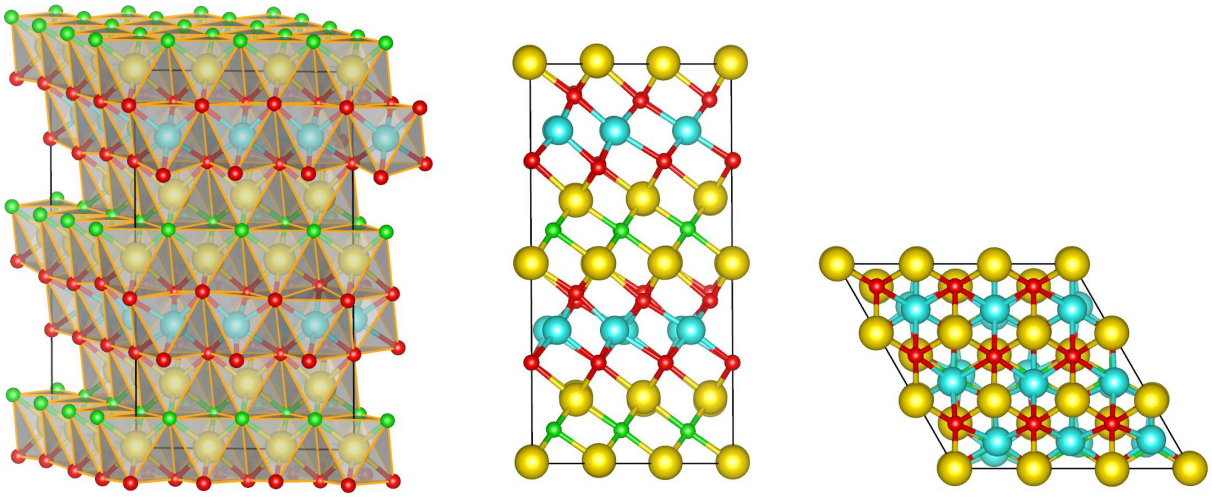

FIG. 1: Structure of the distorted version of layered–like Li_2VO_2F, showing the coordination polyhedra (left) and projections along the a–axis (middle) and the c–axis (right). The slight shift of the V atoms is clearly visible in the projected structures.

Pair distribution function in DRS–type Li_2VO_2F and Li_2VO_3

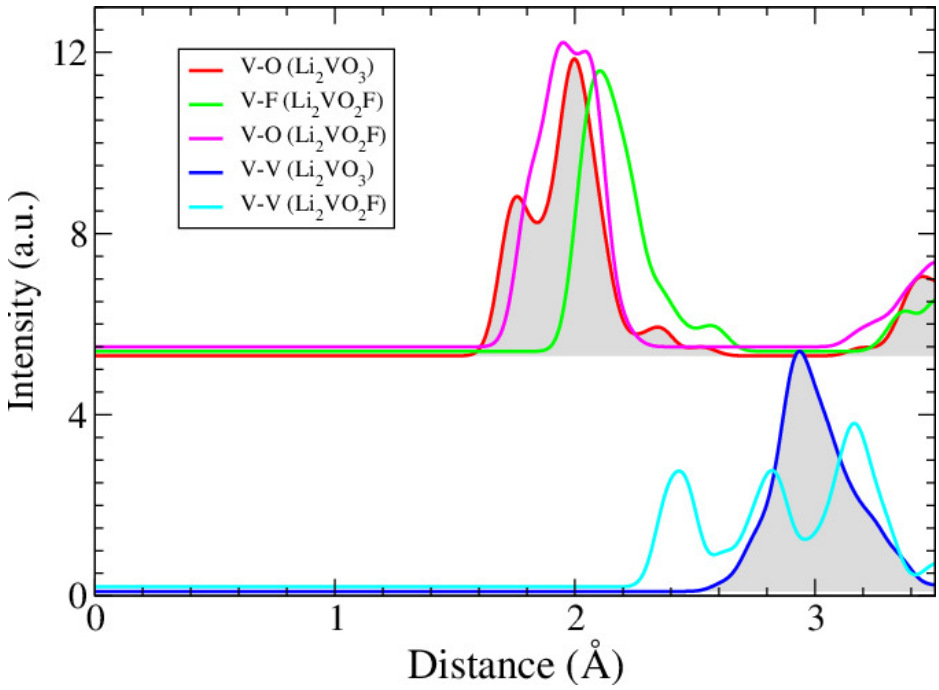

FIG. 2: Pair distribution function of the DRS–type Li_2VO_2F and Li_2VO_3. The increased V–F distances in Li_2VO_2F and the resulting changes in the V distribution are clearly visible from comparison to the DRS oxide.

Di–vacancy diffusion pathways in Li_2VO_2F and Li_2VO_3

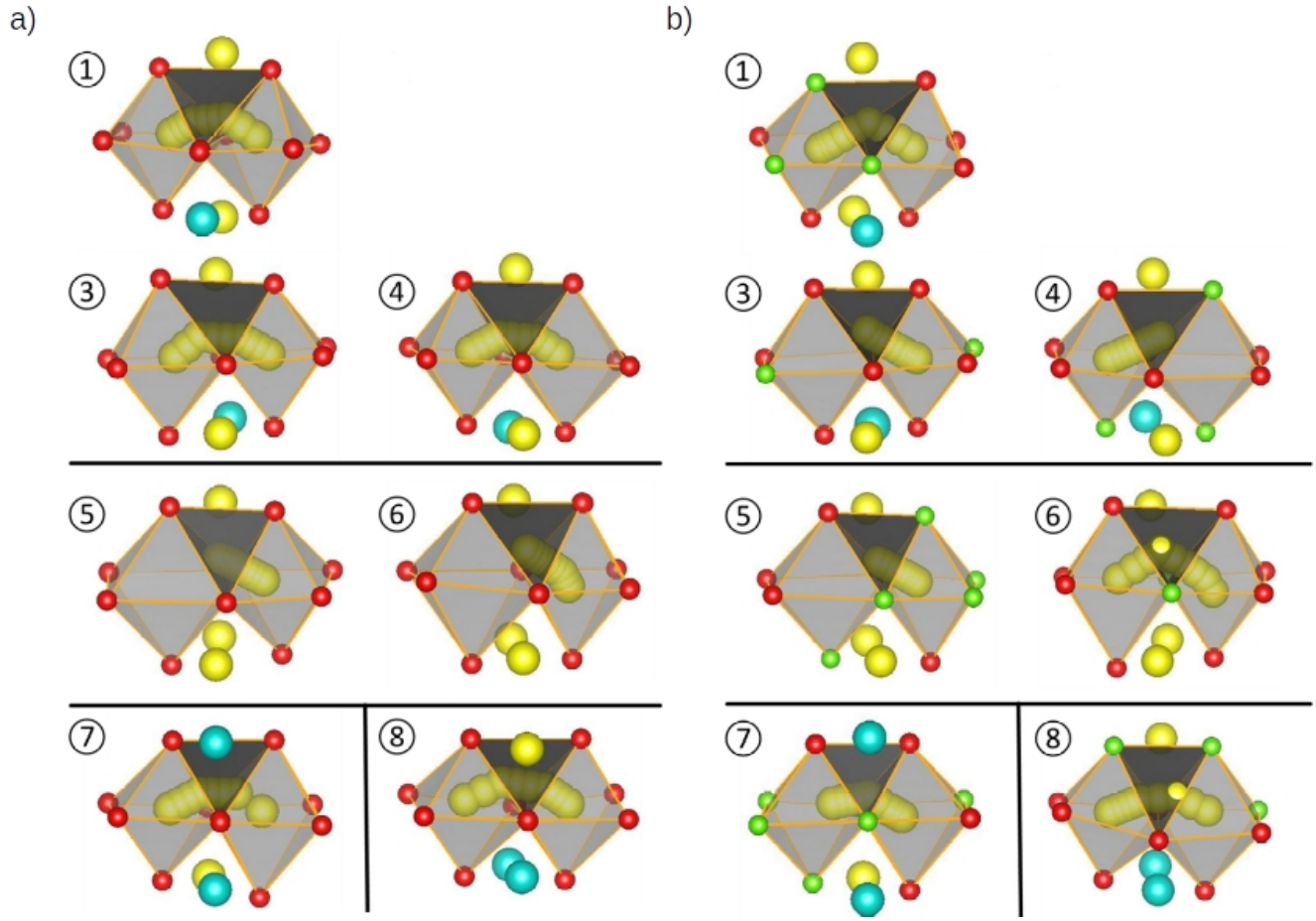

FIG. 3: Di–vacancy diffusion: Diffusion pathways in the presence of di–vacancies for a) Li_2VO_3 and b) Li_2VO_2F (right).