Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Ab initio study of Li, Mg and Al insertion into rutile VO_2: Fast diffusion and enhanced voltages for multivalent batteries

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Supporting information

Table S1. Relative total energies (in meV per formula unit) of FM and AFM VO_2 and Li-VO_2. Zero energy is referenced to FM state

	VO_2	$Li_{0.33}VO_2$	$Li_{0.5}VO_2$	$LiVO_2$
FM	0	0	0	0
AFM	+45	+43	+53	+52

Table S2. Voltage for Li insertion in rutile and monoclinic phases of VO_2

Composition	V (V) (rutile)	V (V) (monoclinic)
$Li_{0.03}VO_2$	-3.50	-3.27
$Li_{0.25}VO_2$	-2.81	-2.59