About the tool:

This is a machine learning tool to efficiently predict the voltage of bulk electrode materials for different metal ion batteries. Users with minimal information about materials, will be able to predict the voltage typically within a minute. It works only for battery electrodes that are based on intercalation chemistry.

User inputs required for prediction:

High ion concentration: Stoichiometry of the electrode material for which you want to predict the voltage of. e.g. $M_{0.75}TiO_2$ or M_1TiO_2. (M = Li, Na, K, Mg, Ca, Al, Zn, Y)

Low ion concentration: Stoichiometry of the electrode material at lower M-ion concentration where you add more M-ions to obtain the higher intercalated material. e.g. $M_{0.50}TiO_2$ or TiO_2

Fraction of M-ion at high concentration: It is the fraction of M-ion in higher concentration of the intercalated material. e.g. $\frac{x}{x+y+z}$ for $M_xTi_yO_z$.

Type of M-ion battery: Specification for a type of battery you want to predict the voltage for. Select from drop down menu.

Crystal lattice type: Specification of crystal lattice type for electrode material. Note that, it is trained to work only for electrodes that does not undergo change in crystal symmetry upon intercalation or de-intercalation.

Space group: Specification of the space group of the electrode material.

Few input examples:

Table 1: Example inputs to get familiar with the tool. Each row corresponds to one complete set of parameters required as input in the order listed above. The output of the tool provides the average voltage (in V) for the electrode in the first column (high ion concentration) with respect to the second column (low ion concentration).

$Ca_{0.5}NiS_2$	NiS_2	0.14286	Ca	triclinic	2
$NaFePO_4$	$FePO_4$	0.14286	Na	orthorhombic	62
$MgVO_3$	$Mg_{0.5}VO_3$	0.20000	Mg	orthorhombic	63