Electronic Supplementary Information for

“Materials with the $CrVO_4$ structure type as candidate superprotonic conductors”

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1. Finding oxidation states and charges

The bond valence-based energy model requires that every atom in the material is assigned a nominal oxidation state. To determine the oxidation states for the elements, we use the following algorithm:

1. For a given structure, list all the likely oxidation states for all the elements in the structure. We used the information from the book Chemistry of the Elements, 2nd Edition by Greenwood and Earnshaw[1] to create this list. We assign a prior likelihood to each oxidation state based on the count of the oxidation state in ICSD[2]. We also checked the rarity for a given oxidation state and incremented (or decremented) the count based on whether the oxidation state is never known before (decrement of 5), rare (increment of 10), or common (increment of 50). The relative counts of each state for a given element allow us to determine the prior probability, $P(oxidation)$, of the element achieving that state.
2. For each atom in the structure, calculate the valence, BV, predicted by the bond-valence method.
3. Let $P(BV\,|\,oxidation)$ be calculated using a Gaussian distribution over the difference between the atomic valence any given oxidation state. The standard deviation of this distribution was set to be 1. We can the calculate the probability of any oxidation state for a given valence using Bayes’ theorem:

$$P(oxidation\,|\,BV) = P(BV\,|\,oxidation)P(oxidation) \tag{1}$$

4. Consider all possible combinations of oxidation states in the structure that preserve charge balance and select the one that maximizes the product of $P(oxidation\,|\,BV)$ over all atoms.

The oxidation states are not necessarily equal to the physical charge at each site, but for simplicity we approximated the effective charge to be proportional to the oxidation state. Thus the effective charge of each site was calculated by multiplying the oxidation state by a constant factor, q_s:

$$q = q_s \times (\text{oxidation state}) \tag{2}$$

The charge scaling factor q_s was one of the parameters fit to DFT calculations.

2. Treatment of solids and relaxation

To take into account the possible relaxation of atoms in the solids, we treat the atoms in the solid as if they are attached to their ideal lattice sites with springs, where the spring constant k is defined as:

$$k = k_0 + k_s \left|q\right| \tag{1}$$

where k_0 is the base value of the spring constant, k_s is a charge-scaling factor, and q is the charge for a given site.

In the presence of a diffuser, an atom is assumed to relax from its ideal site by a distance of r_{offset}. The pair interaction, accounting for relaxations, is then:

$$E_{relax}\left(r\right) = E_{pair}\left(r + r_{offset}\right) + \frac{k}{2}\left(r_{offset}\right)^2 \tag{2}$$

where r is the ideal distance between the atoms.

To find the value of r_{offset} at equilibrium, the force between the two atoms must be zero:

$$0 = \frac{dE_{relax}\left(r\right)}{dr_{offset}} = E_{pair}'\left(r + r_{offset}\right) + kr_{offset} \ . \tag{3}$$

We approximate $E_{pair}'\left(r + r_{offset}\right)$ using Taylor expansion:

$$E_{pair}'\left(r + r_{offset}\right) \approx E_{pair}'\left(r\right) + E_{pair}''\left(r\right) r_{offset} \tag{4}$$

substituting equation (2.4) to equation (2.3):

$$0 = \frac{dE_{relax}\left(r\right)}{dr_{offset}} \approx E_{pair}'\left(r\right) + E_{pair}''\left(r\right) r_{offset} + kr_{offset} \tag{5}$$

$$r_{offset} \approx \frac{-E_{pair}'(r)}{E_{pair}''(r)+k} \quad . \tag{6}$$

The above expression allows us to rapidly estimate the value of r_{offset} and approximately account for atomic relaxation in our energy model.

3. Energy model construction and parameters

To screen for potential proton conductors, we employed a simple energy model that combines an exponential repulsion term backed with a Coulomb screening term:

$$E_{pair} = E_{Exp} + E_{Coulomb} \tag{7}$$

where

$$E_{Coulomb} = k\frac{q_i q_j}{r} e^{\frac{-r}{d}} \tag{8}$$

$$E_{\exp} = Ae^{-rC} . \tag{9}$$

The exponential repulsion term is backed by the bond-valence parameters and model found by Brese and O'Keefe[3]:

$$R_o = r_i + r_j - \frac{r_i r_j (\sqrt{c_i} - \sqrt{c_j})^2}{c_i r_i + c_j r_j} \tag{10}$$

where r_i , r_j , c_i , and c_j are element specific parameters provided by Brese and O'Keefe.

Initial values for the parameters A and C (we will call these A_0 and C_0) were found using the following algorithm:

1. Determine the effective charges for the atoms in the material using the approach described in section 1.
2. For each atom in the structure, calculate the R_o value between that atom and hydrogen from O'Keefe and Brese's parameters and equation. This is the initial R_o and we will call it R_{o_init} .

3. Scale R_{o_init} with a universal scaling factor, r_s , such that $R_{o\_s} = R_{o\_init} r_s$. We scaled the value of R_o because O'Keefe and Brese showed that while the R_o values found from their model show a linear correlation with the real observed bond distances, the value they had for hydrogen is an outlier.[3]
4. For each of the following structure types,
    a. Rhenium trioxide
    b. Cristabolite
    c. Cuprite
    d. Wurtzite (hexagonal)
    e. Rutile
    f. Fluorite
    g. Rock salt
    h. Cesium chloride,

    find the bond valence s_{ij} between anions and cations based on the coordination number.
5. Using the value of s_{ij} and R_{o_s} found above, calculate the ideal r for every given structure using the bond valence relationship, $s_{ij} = \exp\left(\frac{R_o - r}{b}\right)$.
6. Fit A_0 and C_0 by minimizing the difference between the equilibrium bond lengths for the energy model and ideal r values found in step 6. The values for A_0 and C_0 found this way are shown in Table 1-S

Table 1-S. The values of A_0 *and* C_0 for different elements from the algorithm above before scaling factor is applied.

Atomic Number	**Element Name**	A_0 **value (eV)**	C_0 **value (1/Å)**
1	hydrogen	221.9308	6.326371
3	lithium	1488.779	5.987387
4	beryllium	855.2014	6.058016
5	boron	807.1233	6.054705
6	carbon	818.045	6.050931
7	nitrogen	724.9243	6.068031
8	oxygen	575.4666	6.104692
9	fluorine	393.2073	6.164485
11	sodium	12387.92	6.433914
12	magnesium	2926.124	5.907983
13	aluminum	2417.579	5.949664
14	silicon	2304.041	5.935647
15	phosphorus	2172.857	5.932193
16	sulfur	1928.756	5.965598
17	chlorine	1743.925	5.967689
19	potassium	39767.03	6.245923
20	calcium	19687.23	6.363112
21	scandium	10919.34	6.400903
22	titanium	3418.643	5.86216
23	vanadium	3030.132	5.91109
24	chromium	2627.325	5.927545
25	manganese	2682.867	5.913579
26	iron	2615.633	5.917104
27	cobalt	2097.285	5.935246
28	nickel	1802.869	5.951649
29	copper	1065.052	6.02664
30	zinc	1978.228	5.948852
31	gallium	2504.425	5.918385
32	germanium	3047.044	5.909144
33	arsenic	3211.198	5.876663
34	selenium	3107.699	5.899439
35	bromine	2721	5.930455
37	rubidium	20451	5.732408
38	strontium	11571.63	5.771011
39	yttrium	7618.364	5.813256
40	zirconium	13426.42	6.304055
41	niobium	5372.929	5.853688
42	molybdenum	4870.293	5.8563
44	ruthenium	2976.293	5.903065

45	rhodium	2804.601	5.92546
46	palladium	2171.285	5.941574
47	silver	2247.833	5.934706
48	cadmium	3977.844	5.928631
49	indium	12185.16	6.441506
50	tin	5193.418	5.857844
51	antimony	9265.984	6.10237
52	tellurium	17296.56	6.384611
53	iodine	4866.394	5.851438
55	cesium	105654.4	6.104346
56	barium	23628.27	5.731376
57	lanthanum	37704.82	6.250221
58	cerium	12127.21	5.756003
59	praseodymium	11849.48	5.780223
60	neodymium	10987.64	5.778148
62	samarium	10245.66	5.798301
63	europium	10392.85	5.789439
64	gadolinium	9151.173	5.794684
65	terbium	9149.794	5.832182
66	dysprosium	8339.335	5.822479
67	holmium	9062.617	5.883528
68	erbium	7322.257	5.811325
69	thulium	7133.626	5.816795
70	ytterbium	6862.874	5.818053
71	lutetium	17959.58	6.379059
72	hafnium	15323.36	6.399602
73	tantalum	5506.245	5.883319
74	tungsten	5085.098	5.851917
75	rhenium	4922.541	5.849618
77	iridium	4992.275	5.850301
80	mercury	4271.098	5.874973
81	thallium	11094.77	5.795774
82	Lead	8600.042	5.826843
83	bismuth	8769.27	5.808584
90	thorium	14500.64	5.80836
92	uranium	9543.9	5.79126

For cation-cation interactions, the value of A was calculated by multiplying A_0 by a universal scaling constant a_s:

$$A = A_0 a_s \tag{11}$$

For anion-cation interactions, we did not scale the value of A. A similar approach was used for C. For an anion-cation interaction:

$$C_{eff} = \frac{C}{a_c} \tag{12}$$

and for a cation-cation interaction

$$C_{eff} = c_c C \tag{13}$$

Altogether, there are eight parameters (such as the scaling factors) for the energy model that were determined by fitting to DFT-calculated activation energies of a training set of 52 materials. The list of eight parameters and their final values are shown in Table *2*-S, and the training data are summarized in Table 3-S.

Table 2-S. Parameters used in the model and their values after fitting. q_e is the elementary charge.

Symbol	**Parameter**	**Value**	**Unit**
k_0	Spring constant base value	5	eV / Å^2
k_s	Spring constant scaling	4	eV / (q_e Å^2)
d	Screening radius for Coulomb interaction	0.71	Angstrom
q_s	Charge scaling	0.42	
a_s	Cation-cation scaling term for A	0.83	
a_c	Anion-cation scaling term for C	0.79	
c_c	Cation-cation scaling term for C	0.90	
r_s	Universal R_o-value scale	0.91	

Fitting to DFT calculations was done incrementally using a grid search using the Pearson correlation coefficient as the primary metric after accounting for outliers identified using the average error and standard deviation of the predicted values. We started with the cubic perovskite crystal class, then added hexagonal perovskite, spinel, elpasolite and other randomly selected structure. Through this method we were able to rapidly identify a good region of parameter space and then refine our values. The outcome of the final fitting process for the 52 training structures is shown in Table 3-S:

Table 3-S. The 52 structures used to train the model.

Composition	**Oxide Structure Type**	**Model Predicted Activation Energy (eV)**	**DFT+NEB Calculated Activation Energy (eV)**	**Absolute Difference (eV)**
Ca_2MgWO_6	Alternating Perovskite	0.416737	0.564008	0.147271
$CrSrO_3$	Cubic Perovskite	0.25348	0.19972	0.053759
$CaTiO_3$	Cubic Perovskite	0.317002	0.46147	0.144468
$MoSrO_3$	Cubic Perovskite	0.386586	0.599814	0.213228
$KTaO_3$	Cubic Perovskite	0.409248	0.386502	0.022745
$GePbO_3$	Cubic Perovskite	0.293683	0.3292	0.035517
$CaSiO_3$	Cubic Perovskite	0.426016	0.37739	0.048626
$NaWO_3$	Cubic Perovskite	0.294477	0.230381	0.064096
$KCrO_3$	Cubic Perovskite	0.375982	0.309166	0.066816
$SrZrO_3$	Cubic Perovskite	0.469067	0.741086	0.272019
$BaTiO_3$	Cubic Perovskite	0.369738	0.249483	0.120255
$BaZrO_3$	Cubic Perovskite	0.502707	0.27732	0.225387
$BaIrO_3$	Cubic Perovskite	0.439164	0.378972	0.060192
$BaSnO_3$	Cubic Perovskite	0.463129	0.179522	0.283607
$BaPbO_3$	Cubic Perovskite	0.556238	0.266042	0.290196
$SrNbO_3$	Cubic Perovskite	0.412975	0.330074	0.082901
$BaNbO_3$	Cubic Perovskite	0.435342	0.251341	0.184001
$LaAlO_3$	Cubic Perovskite	0.230819	0.287421	0.056601
$SrTiO_3$	Cubic Perovskite	0.335922	0.189221	0.1467
$Ba_2NiO6Re$	Elpasolite	0.737628	0.580371	0.157257
GaO_6SbSr_2	Elpasolite	0.567261	0.514962	0.052299
Ba_2MgWO_6	Elpasolite	0.546621	0.532571	0.01405
Ba_2FeMoO_6	Elpasolite	0.507778	0.578513	0.070736
Ba_2FeReO_6	Elpasolite	0.458289	0.546507	0.088218
Ba_2ZnReO_6	Elpasolite	0.486157	0.48288	0.003277
Ba_2CoReO_6	Elpasolite	0.577129	0.480684	0.096445
Ba_2MoNiO_6	Elpasolite	0.467585	0.495648	0.028063
$BaSiO_3$	Hexagonal Perovskite	0.479127	0.87437	0.395243
$BaNiO_3$	Hexagonal Perovskite	0.773659	0.810901	0.037242
$BaRuO_3$	Hexagonal Perovskite	0.776816	0.464395	0.312421

$BaCoO_3$	Hexagonal Perovskite	0.968349	0.855273	0.113075
$LaCrO_3$	Hexagonal Perovskite	0.26082	0.363617	0.102797
$Si_2Sc_2O_7$	Pyrocholre	0.388962	0.40772	0.018758
SiO_2	Quartz	0.123985	0.499558	0.375574
Rh_2ZnO_4	Spinel	0.369029	0.330071	0.038958
Rh_2MgO_4	Spinel	0.360327	0.258765	0.101562
Rh_2CoO_4	Spinel	0.357971	0.333853	0.024119
Ni_2SiO_4	Spinel	0.234994	0.112817	0.122177
Al_2MgO_4	Spinel	0.249057	0.132738	0.116319
Rh_2CdO_4	Spinel	0.580161	0.756126	0.175965
$MgTi_2O_4$	Spinel	0.277899	0.620978	0.343079
CdV_2O_4	Spinel	0.582393	0.452657	0.129736
$GeCo_2O_4$	Spinel	0.266736	0.203161	0.063575
Cr_2CdO_4	Spinel	0.347283	0.362269	0.014986
$CdIn_2O_4$	Spinel	0.664341	0.375366	0.288975
$AlNi_2O_4$	Spinel	0.967221	0.984806	0.017585
$ZnAl_2O_4$	Spinel	0.220391	0.210962	0.00943
Mg_2VO_4	Spinel	0.348982	0.105376	0.243606
Ga_2ZnO_4	Spinel	0.307155	0.334726	0.027571
$CaFeO_3$	Tilted Perovskite	0.345664	0.30236	0.043304
$BaNbO_2$	Zircon	0.131521	0.430281	0.298761

The simple energy model allows for analytical derivatives, which we use to calculate the gradient and Hessian matrix of the potential energy surface at every point on a regular three dimensional grid. From each point on this grid we use gradient descent to identify a nearby stationary point, at which the magnitude of the gradient is zero. We then evaluate the eigenvalues of the Hessian matrix to identify whether the stationary point is a saddle point. From each saddle point gradient descent on the potential energy surface is used to identify the endpoints of a hop that passes through that saddle point. The set of possible hops is completed by applying symmetry operations to all known hops and linking sites that are close together (within 1 Angstrom) but are not already connected by a hop. We evaluate all pathways through the diffusion hop network that start at the site predicted to have the lowest energy and end at a translationally equivalent site. The path for which the maximum energy along the path is lowest is used to calculate the migration energy, which is simply defined as the difference between the highest and lowest energy points along the path.

4. Band gaps and DFT+U calculations

In this section we show the calculated band gaps and the results of proton migration barriers using DFT+U and compared to the results without +U in the main text (Table 2). The DFT+U calculations were performed for $CrVO_4$-structured oxides that contain elements of Co, Cr, Fe, Mn, Ni, and V (Table 4-S). The U parameters were chosen according to Wang et al.[4] by fitting to experimental formation enthalpies. We have used the POTCAR files used by the Materials Project for the oxides containing Fe and Ni, because the DFT+U calculations had difficulty converging for these materials using the GW PAW POTCAR files we used in the rest of this work. The band gaps with and without DFT+U were calculated in the same way as other DFT calculations (see the Methodology section in the main text), followed by a static calculation by setting ICHARG=11 in VASP and using the charge density from the previously converged self-consistent run.

Table 4-S. Proton migration activation barrier and band gap for all 29 $CrVO_4$-structured oxides without and with DFT+U.

ICSD ID	Composition	DFT Activation Barrier without / with U (eV)	U value (eV)	Band gap without / with U (eV)
16618	$InPO_4$	0.340 / -	-	2.51 / -
16619	$TlPO_4$	0.270 / -	-	1.21 / -
16741*	$NiSO_4$	0.187 / 0.183	Ni: 6.2	3.97 / 4.93
16759	$MgSO_4$	0.234 / -	-	4.52 / -
18117	$MgCrO_4$	0.094 / 0.065	Cr: 3.7	2.15 / 2.49
18118	$CdCrO_4$	0.056 / 0.056	Cr: 3.7	2.03 / 2.31
23492	$CoCrO_4$	0.094 / 0.204	Co: 3.32, Cr: 3.7	0.03 / 1.51
23493*	$NiCrO_4$	0.053 / 0.061	Ni: 6.2, Cr: 3.7	0.71 / 1.92
23507*	$FeSO_4$	0.164 / 0.187	Fe: 5.3	2.12 / 4.07
25700*	$NiSeO_4$	0.188 / 0.209	Ni: 6.2	1.07 / 2.37
31231	$MnSO_4$	0.217 / 0.190	Mn: 3.9	2.60 / 3.86
33736	$CoSO_4$	0.229 / 0.235	Co: 3.32	3.40 / 4.53
36244	$CrVO_4$	0.172 / 0.100	V: 3.25, Cr: 3.7	0.52 / 1.79
60571	$CdSO_4$	0.177 / -	-	3.34 / -
62159	$CrPO_4$	0.242 / 0.326	Cr: 3.7	0.68 / 1.88
82282	$TiPO_4$	0.321 / -	-	0.01 / -
82286	VPO_4	0.196 / 0.188	V: 3.25	0.00 / 1.65
82161*	$FeVO_4$	0.129 / 0.102	V: 3.25, Fe: 5.3	0.03 / 3.11
89505	$LiMnO_4$	0.086 / 0.072	Mn: 3.9	1.32 / 1.53
109070	$MgSeO_4$	0.282 / -	-	2.87 / -
109071	$MnSeO_4$	0.165 / 0.226	Mn: 3.9	0.06 / 1.57
109072	$CoSeO_4$	0.256 / 0.195	Co: 3.32	0.57 / 2.00
109073	$CuSeO_4$	0.295 / -	-	1.35 / -
155065*	$FePO_4$	0.171 / 0.220	Fe: 5.3	0.03 / 5.07
155162	$InVO_4$	0.054 / 0.055	V: 3.25	3.02 / 3.12
159272	$AlPO_4$	0.161 / -	-	5.78 / -
166436	$TiSiO_4$	0.091 / -	-	1.54 / -
183216	$CuCrO_4$	0.154 / 0.089	Cr: 3.7	1.10 / 1.38
416147	$HgCrO_4$	0.085 / 0.073	Cr: 3.7	1.39 / 1.46

*These calculations were performed using the pseudopotential files used by the Materials Project.

5. VASP PAW potentials

Table 5-S provides a list of the VASP PAW potentials used in this work for each element.

Table 5-S. VASP PAW potentials used for each element.

Element	Pseudopotential
Ac	PAW_PBE Ac 06Sep2000
Ag	PAW Ag_GW 06Mar2008
Al	PAW Al_GW 19Mar2012
Am	PAW_PBE Am 08May2007
Ar	PAW Ar_GW 02Oct2006
As	PAW As_GW 20Mar2012
At	PAW At 21May2007
Au	PAW Au_GW 23Mar2010
B	PAW B 28Sep2005
Ba	PAW Ba_sv_GW 23Mar2010
Be	PAW Be_GW 04Mar2008
Bi	PAW Bi_GW 07Mar2011
Br	PAW_PBE Br 20Mar2012
C	PAW C_GW_new 19Mar2012
Ca	PAW Ca_sv_GW 31Mar2010
Cd	PAW Cd_f_GW 18May2010
Ce	PAW Ce_GW 26Mar2009
Cl	PAW Cl_GW 19Mar2012
Cm	PAW_PBE Cm 17Jan2011
Co	PAW Co_GW 31Mar2010
Cr	PAW_PBE Cr 06Sep2000
Cs	PAW Cs_sv_GW 23Mar2010
Cu	PAW Cu_GW 19May2006
Dy	PAW_PBE Dy 23Dec2003
Er	PAW_PBE Er 01Sep2006
Eu	PAW_PBE Eu 23Dec2003
F	PAW F_GW 19Mar2012
Fe	PAW Fe_GW 31Mar2010
Fr	PAW_PBE Fr_sv 29May2007
Ga	PAW Ga_GW 22Mar2012
Gd	PAW_PBE Gd 23Dec2003
Ge	PAW Ge 04Okt2005
H	PAW H_GW 21Apr2008
He	PAW He_GW 13May2007
Hf	PAW_PBE Hf 20Jan2003
Hg	PAW_PBE Hg_sv_GW 16Apr2014

Ho	PAW_PBE Ho 23Dec2003
I	PAW_PBE I_GW 12Mar2012
In	PAW_PBE In 08Apr2002
Ir	PAW_PBE Ir 06Sep2000
K	PAW K_sv_GW 31Mar2010
Kr	PAW Kr_GW 02Oct2006
La	PAW_PBE La 06Sep2000
Li	PAW Li_GW 11May2007
Lu	PAW_PBE Lu 23Dec2003
Mg	PAW Mg_GW 13Apr2007
Mn	PAW Mn_GW 31Mar2010
Mo	PAW_PBE Mo 08Apr2002
N	PAW N_GW_new 19Mar2012
Na	PAW_PBE Na 08Apr2002
Nb	PAW Nb_sv_GW 23Mar2010
Nd	PAW_PBE Nd 23Dec2003
Ne	PAW Ne_GW 02Oct2006
Ni	PAW Ni_GW 31Mar2010
Np	PAW_PBE Np 06Sep2000
O	PAW O_GW 19Mar2012
Os	PAW_PBE Os 17Jan2003
P	PAW P_GW 19Mar2012
Pa	PAW_PBE Pa 07Sep2000
Pb	PAW_PBE Pb 08Apr2002
Pd	PAW Pd_GW 06Mar2008
Pm	PAW_PBE Pm 23Dec2003
Po	PAW_PBE Po 10Feb2004
Pr	PAW_PBE Pr 23Dec2003
Pt	PAW Pt_GW 10Mar2009
Pu	PAW_PBE Pu 06Sep2000
Ra	PAW_PBE Ra_sv 29May2007
Rb	PAW Rb_sv_GW 23Mar2010
Re	PAW_PBE Re 17Jan2003
Rh	PAW Rh_GW 06Mar2008
Rn	PAW_PBE Rn 28Aug2006
Ru	PAW_PBE Ru 04Feb2005
S	PAW S_GW 19Mar2012
Sb	PAW Sb_GW 21Mar2012
Sc	PAW_PBE Sc 04Feb2005
Se	PAW Se_GW 20Mar2012
Si	PAW Si_GW 19Mar2012
Sm	PAW_PBE Sm 23Dec2003
Sn	PAW_PBE Sn 08Apr2002

Sr	PAW Sr_sv_GW 23Mar2010
Ta	PAW_PBE Ta 17Jan2003
Tb	PAW_PBE Tb 23Dec2003
Tc	PAW_PBE Tc 04Feb2005
Te	PAW Te_GW 22Mar2012
Th	PAW_PBE Th 07Sep2000
Ti	PAW_PBE Ti 08Apr2002
Tl	PAW_PBE Tl 08Apr2002
Tm	PAW_PBE Tm 23Dec2003
U	PAW_PBE U 06Sep2000
V	PAW_PBE V 08Apr2002
W	PAW_PBE W 08Apr2002
Xe	PAW Xe_GW 08Jan2009
Y	PAW Y_sv_GW 23Mar2010
Yb	PAW_PBE Yb 23Dec2003
Zn	PAW Zn_GW 09Oct2010
Zr	PAW Zr_sv_GW 07Apr2010

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