Supporting Information for:

FEFOS: A method to derive oxide formation energies from oxidation states

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1. Additional data

To analyze the breadth of structure morphologies considered by the FEFOS predictions in Figure 2b, we have analyzed the distribution of space groups of the respective sets of oxides to determine whether the conditioned oxides span a more restricted set of morphologies than the structures which are filtered based on morphology. The resulting analyses are shown in Figure S1.

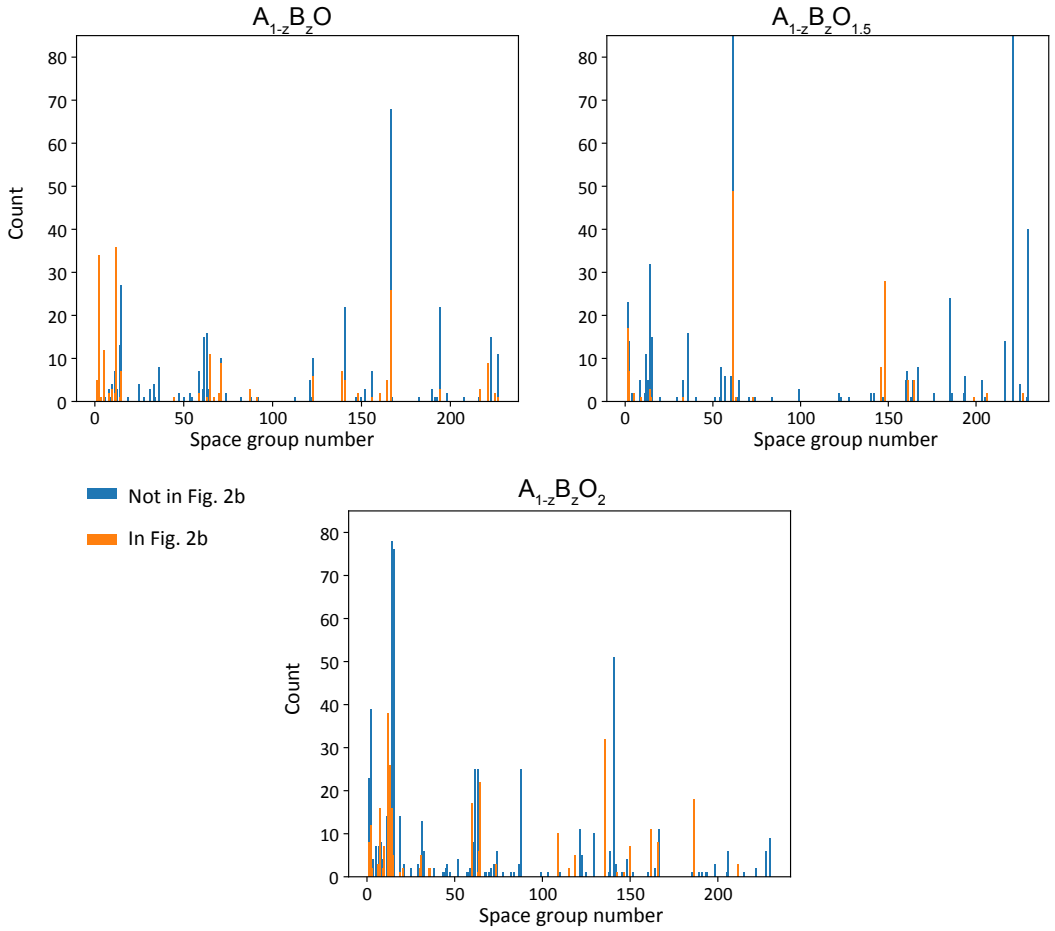


Figure S1. Histogram of space group numbers for each class of oxide considered with assumed overall oxidation numbers of a) 2, b) 3 and c) 4. Counts in blue represent those oxides which were deemed not suitable for formation energy prediction by FEFOS since the oxide did not have the correct coordinations of oxygen and non-oxygen atoms. The counts in blue make up all the points that are plotted in Figure 2b for each class of oxide.

2. Quadratic equation fitting

To construct the datapoints, we set the reference 0 of formation energy to the $\Delta E_{f(MO_y)}$ for the appropriate oxide. We then calculate the difference between $\Delta E_{f(MO_y)}$ and all the ground state formation energies for every other stoichiometry. If the oxygen content of the oxide is higher than it is for MO_y it may be fit through to form f_{ox,MO_y}, while if it is lower, it may be fit through to form f_{red,MO_y}. The x-axis of the datapoints we fit through is determined by the stoichiometry, so that for a perspective MO_c the x-axis value would be set to $2c$. If there is a formation energy which is lower than the reference formation energy MO_y, we simply fit through this point such that the parabola that is formed is symmetric about that minimum.

If the fitted parabola is concave, this is unphysical, since it implies that in the limit of x, oxidation state change, going to infinity, the formation energy would tend to negative infinity. Therefore, we delete the coefficient a_1 and preserve the structure of the parabola close to $x = 0$.

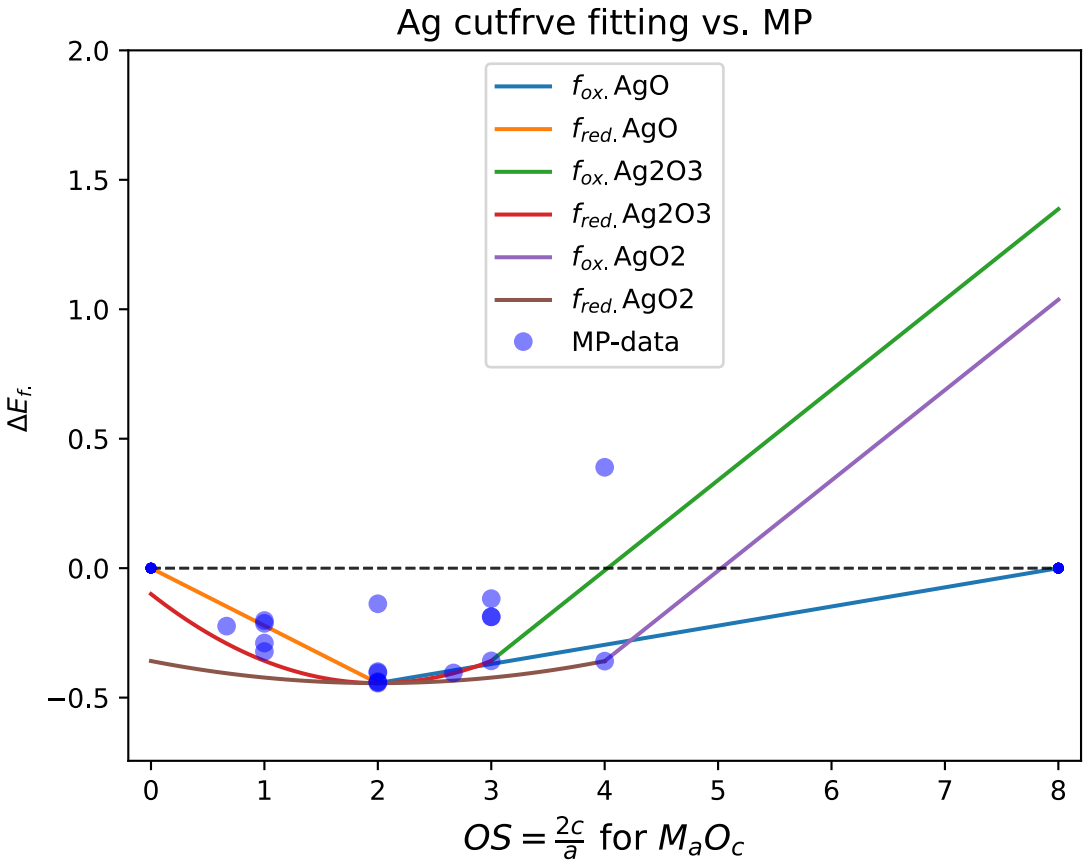
If we cannot fit a quadratic equation because there is not enough data, we simply define linear equations:

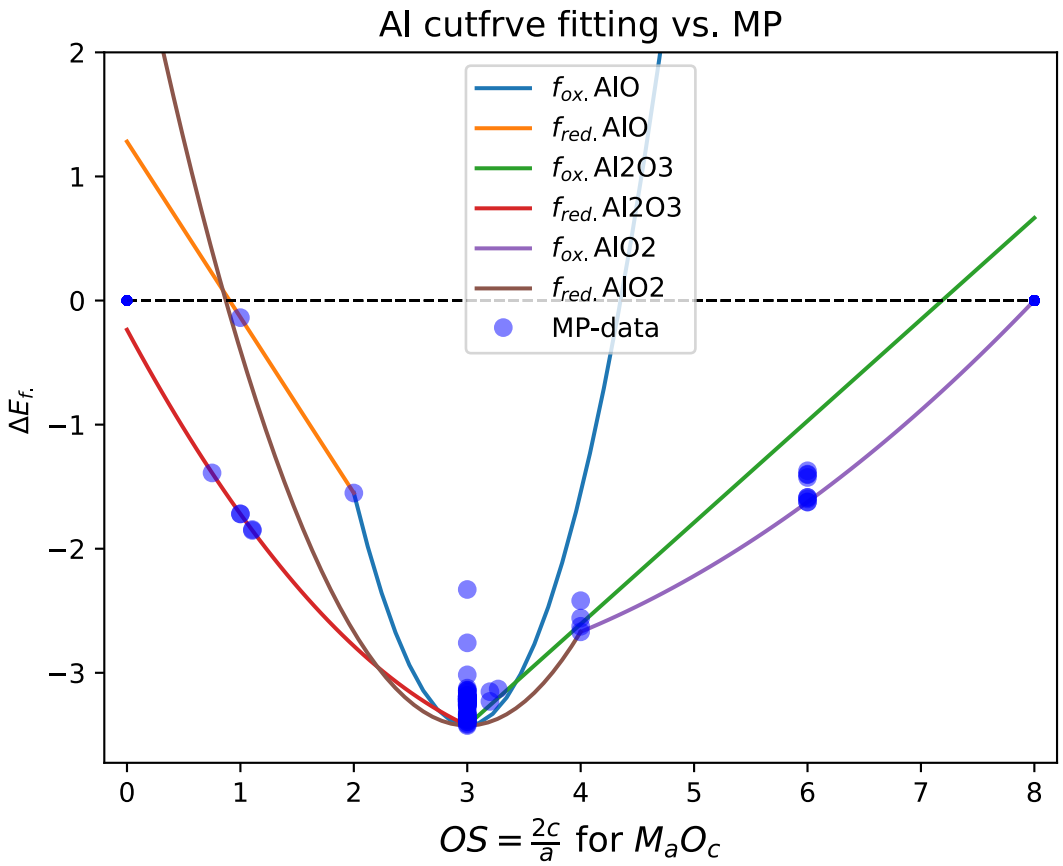
$$f_{red,AO_y} = \frac{\Delta E_{f(AO_y)} x}{ox.state}; \quad f_{ox,AO_2} = \frac{\Delta E_{f(AO_y)} x}{8 - ox.state} \tag{1}$$

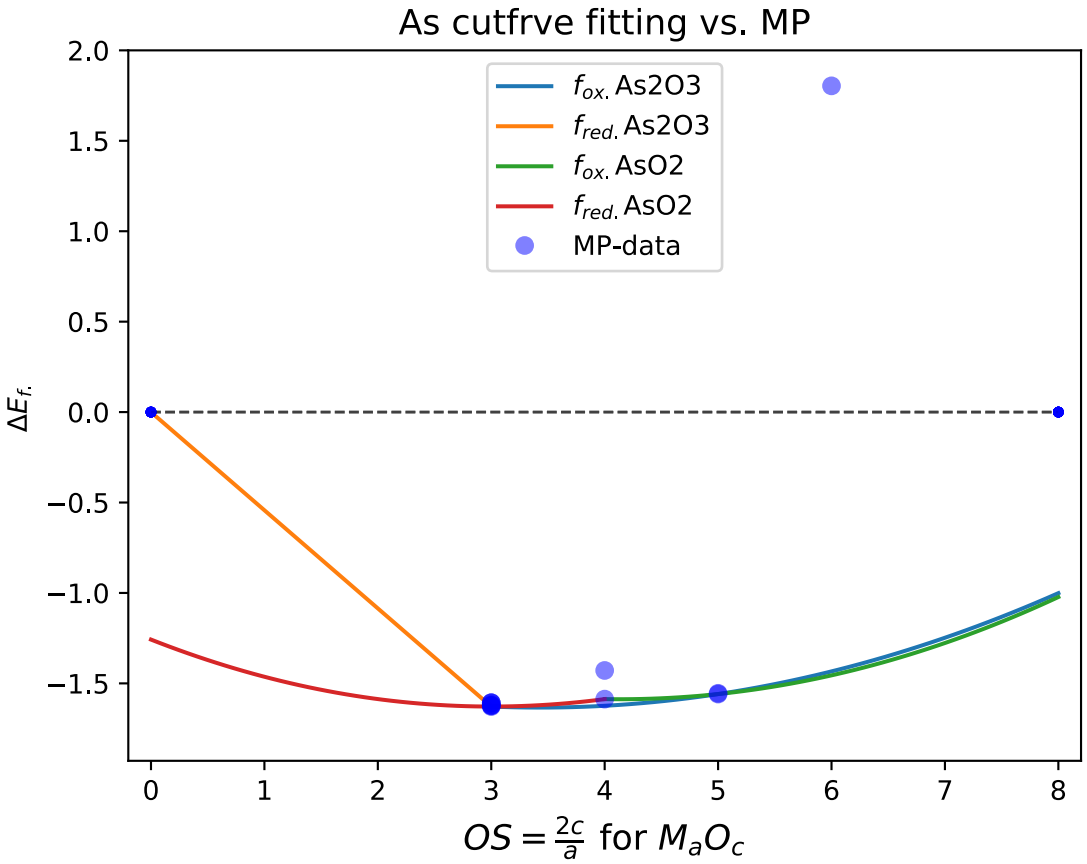
The definition of f_{ox,AO_2} assumes the creation of a more oxidized hypothetical AO_4 material with oxidation state 8+, which is poorly defined, so systems using these linear equations should be treated with relatively more suspicion. This choice is somewhat arbitrary, and effectively comes down to choosing at what oxidation state do we set the formation energy to 0; normally we use the energy of O_2 as the endmember, although this would have an 'infinite' oxidation number as per our oxidation state scheme. Thus, we choose 8+ since it is close to the highest observed oxidation

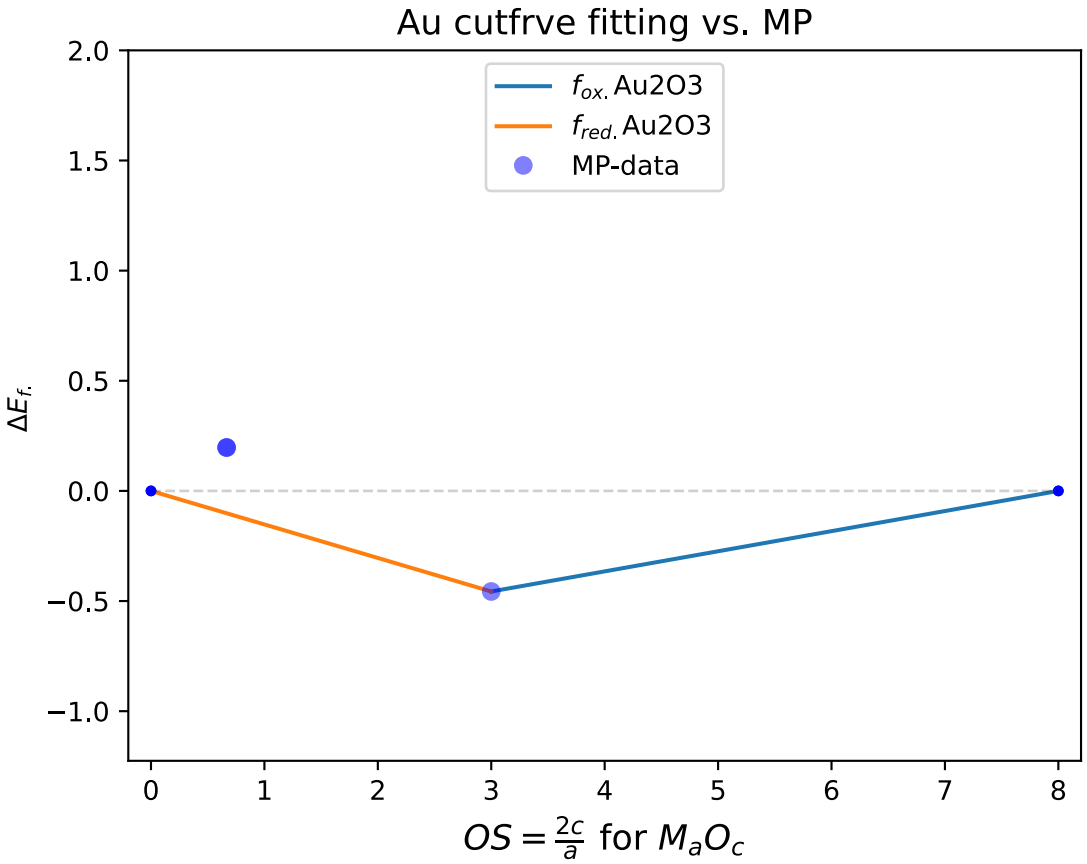
number of 9+,[3] and since it means the denominator of the Eqs. in 1 are the same, affording a symmetry to the equations formed. Future work could focus on tuning this value.

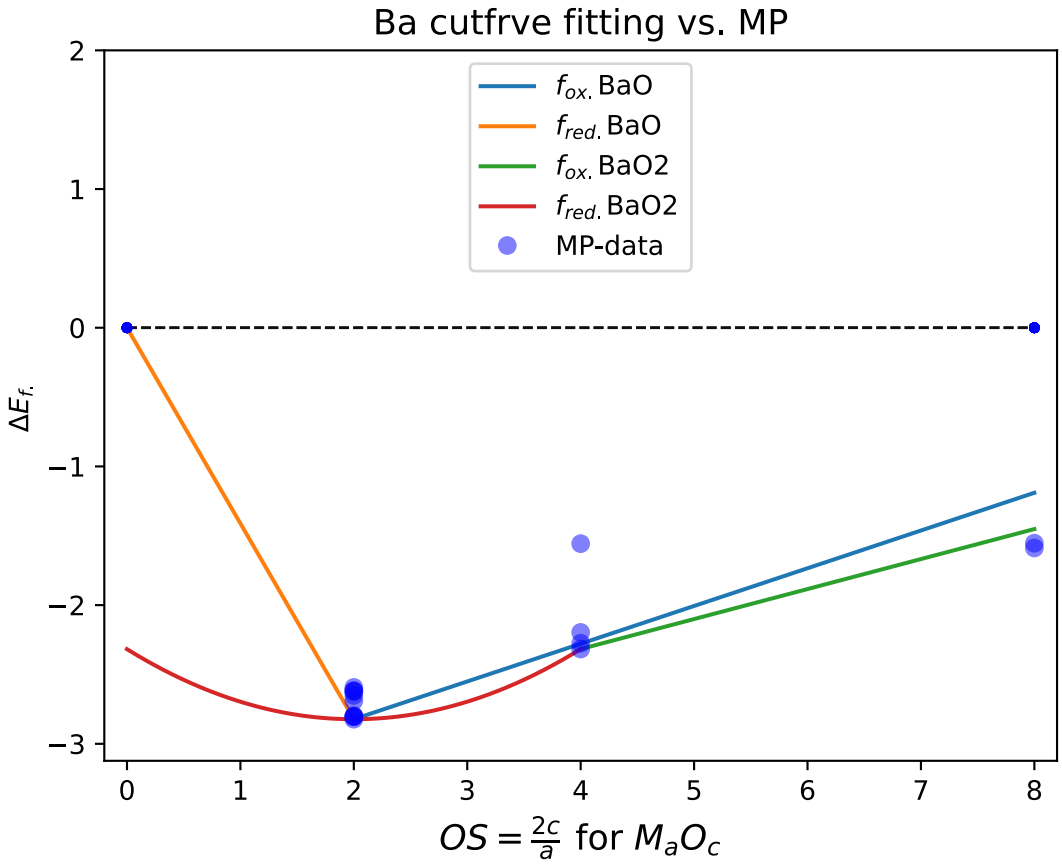
The resultant coefficients can be seen for each element in the plots shown in the following pages.

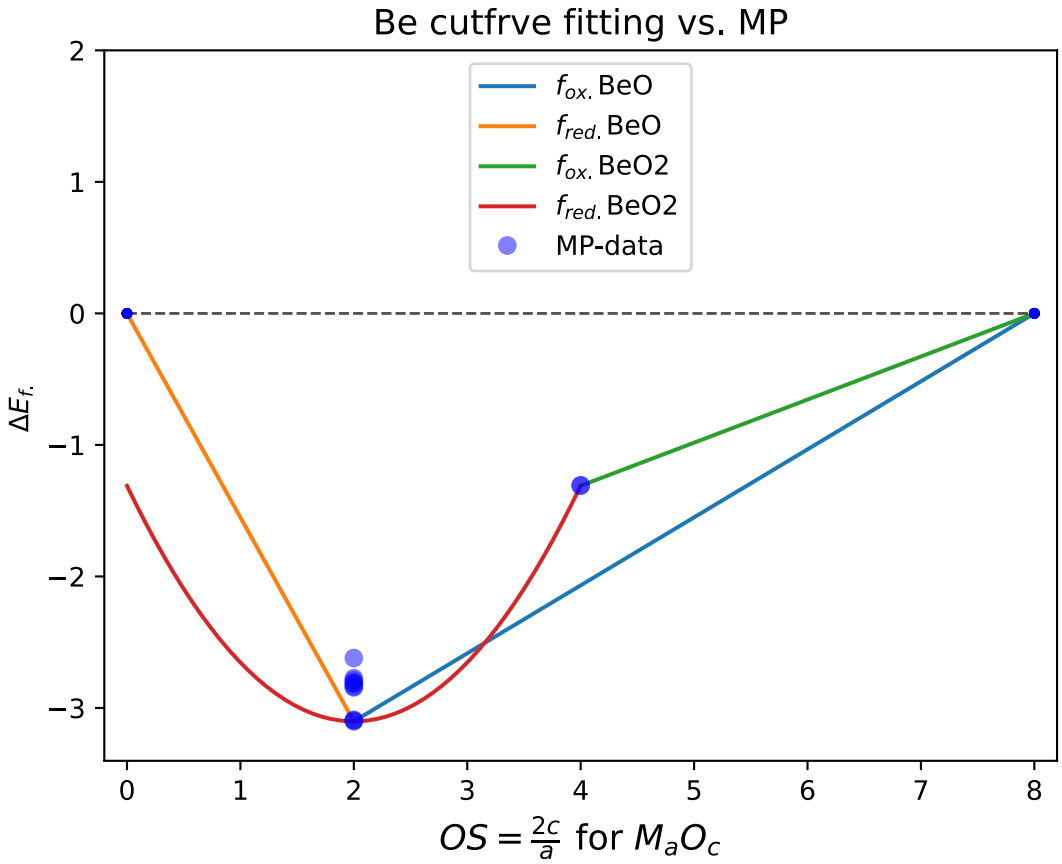

Ag cutfrve fitting vs. MP
$f_{ox.}$ AgO
$f_{red.}$ AgO
$f_{ox.}$ Ag2O3
$f_{red.}$ Ag2O3
$f_{ox.}$ AgO2
$f_{red.}$ AgO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

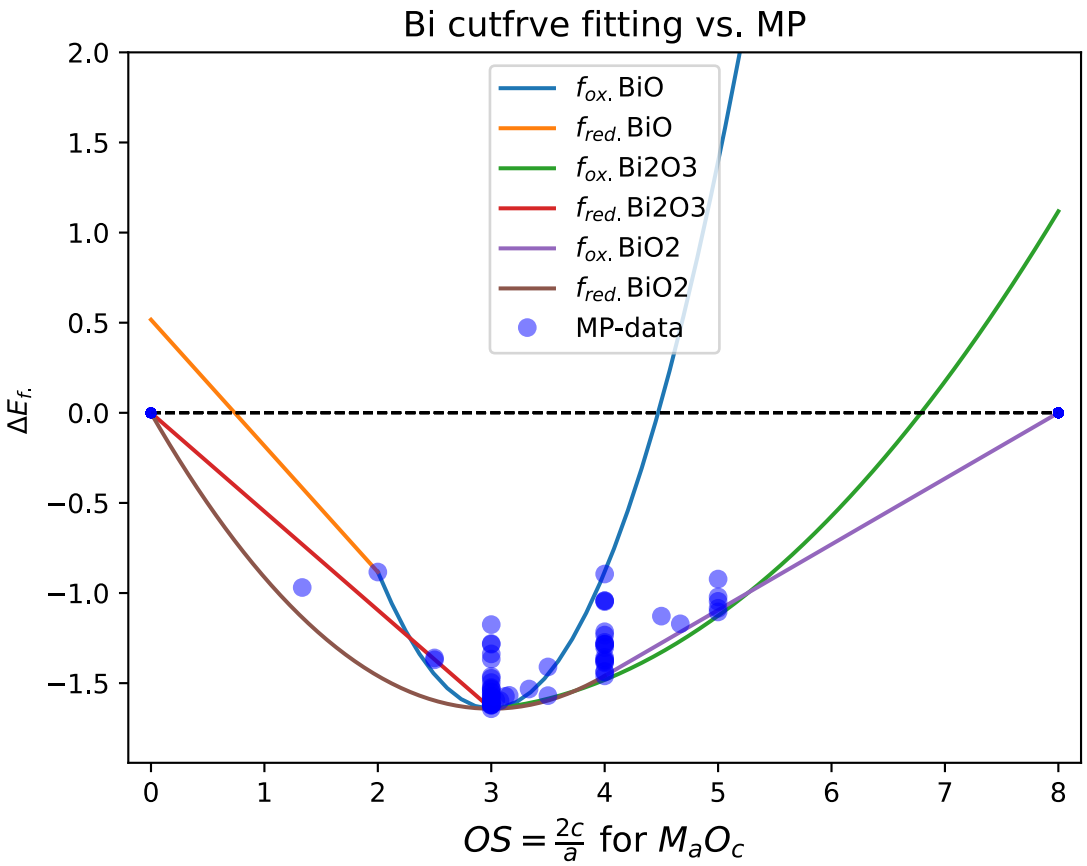

Al cutfrve fitting vs. MP
$f_{ox.}$ AlO
$f_{red.}$ AlO
$f_{ox.}$ Al2O3
$f_{red.}$ Al2O3
$f_{ox.}$ AlO2
$f_{red.}$ AlO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

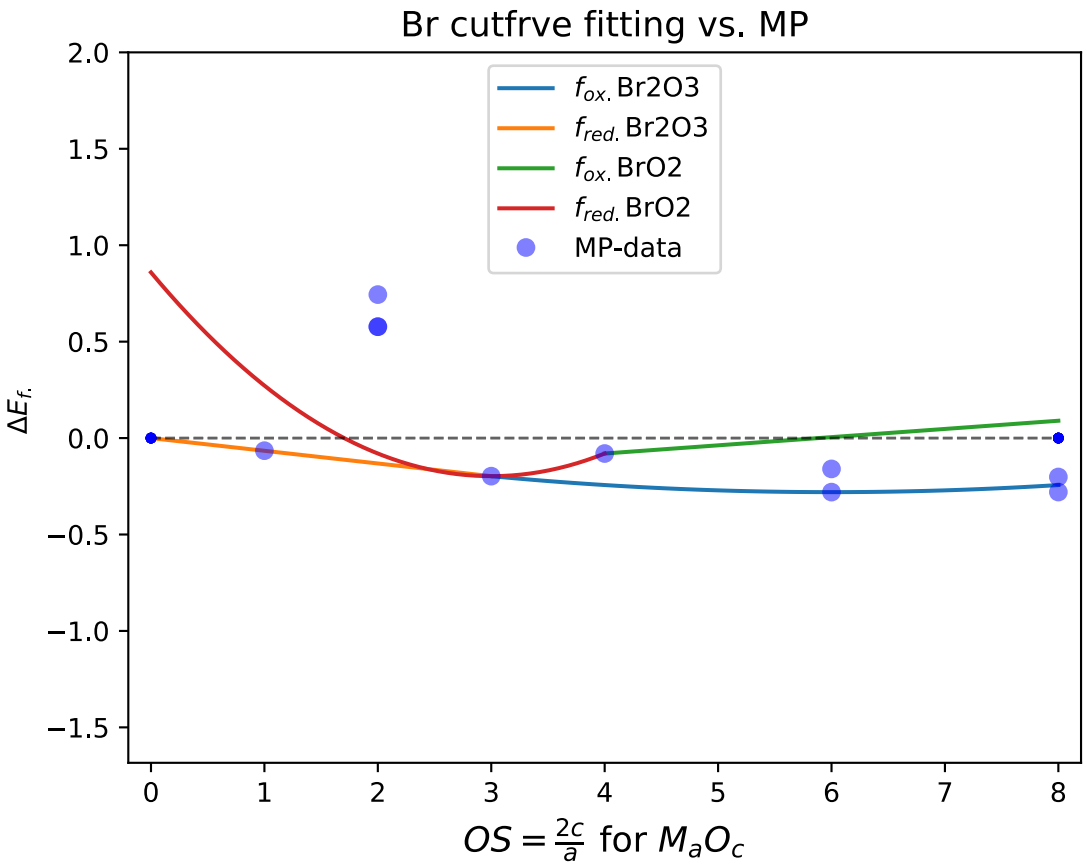

As cutfrve fitting vs. MP
$f_{ox.}$ As2O3
$f_{red.}$ As2O3
$f_{ox.}$ AsO2
$f_{red.}$ AsO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

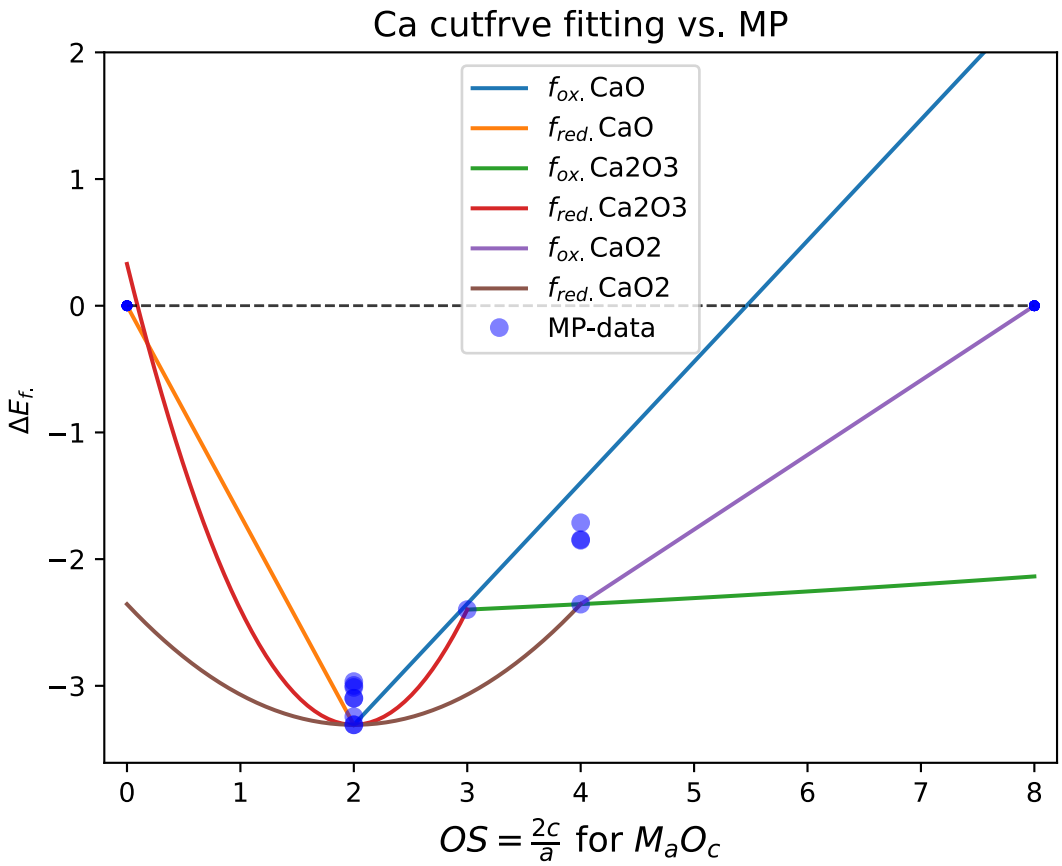

Au cutfrve fitting vs. MP
$f_{ox.}$ Au2O3
$f_{red.}$ Au2O3
MP-data
$\Delta E_{f.}$
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
0
1
2
3
4
5
6
7
8
$OS = \frac{2c}{a}$ for M_aO_c

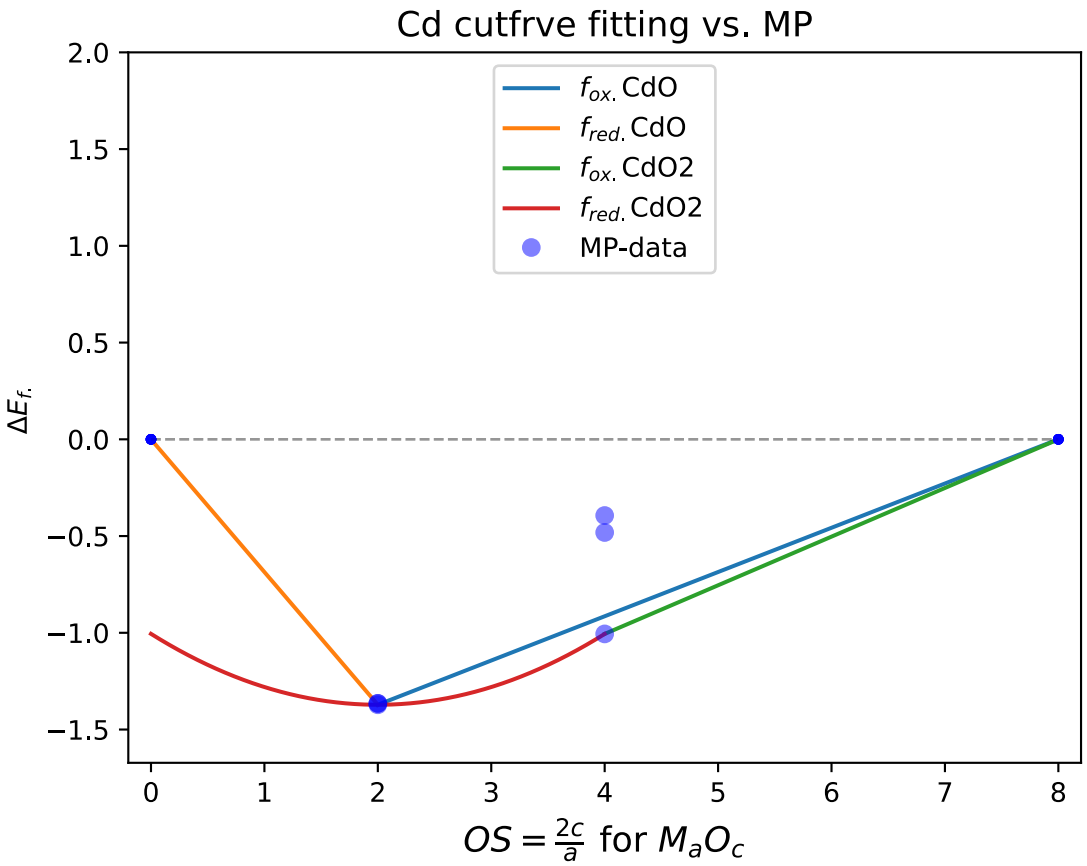

Ba cutfrve fitting vs. MP
$f_{ox.}$ BaO
$f_{red.}$ BaO
$f_{ox.}$ BaO2
$f_{red.}$ BaO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

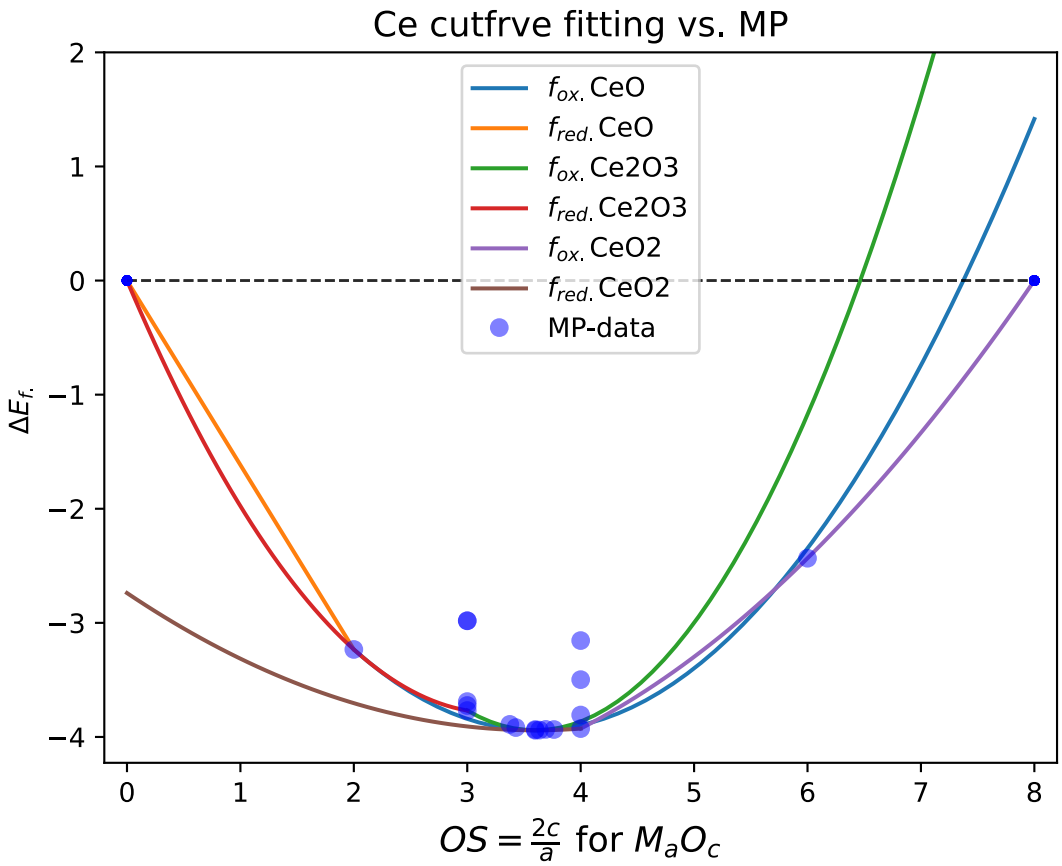

Be cutfrve fitting vs. MP
$f_{ox.}$ BeO
$f_{red.}$ BeO
$f_{ox.}$ BeO2
$f_{red.}$ BeO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

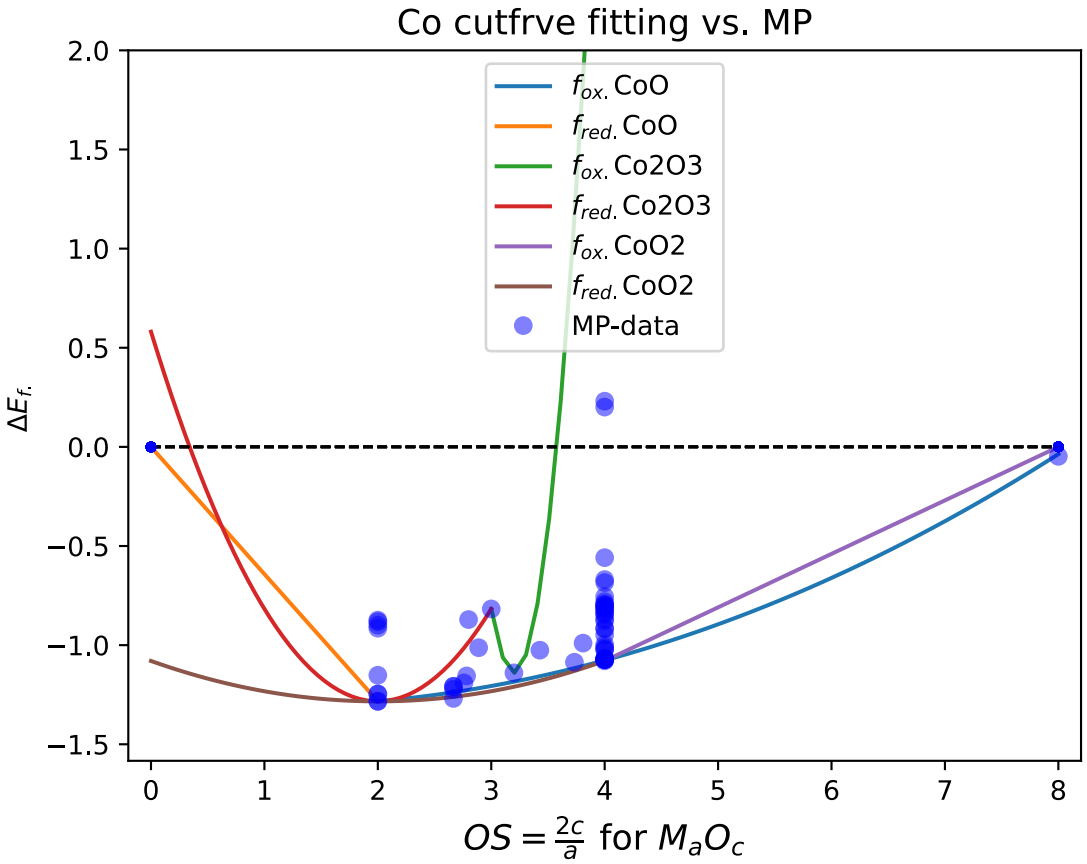

Bi cutfrve fitting vs. MP
$f_{ox.}$ BiO
$f_{red.}$ BiO
$f_{ox.}$ Bi2O3
$f_{red.}$ Bi2O3
$f_{ox.}$ BiO2
$f_{red.}$ BiO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

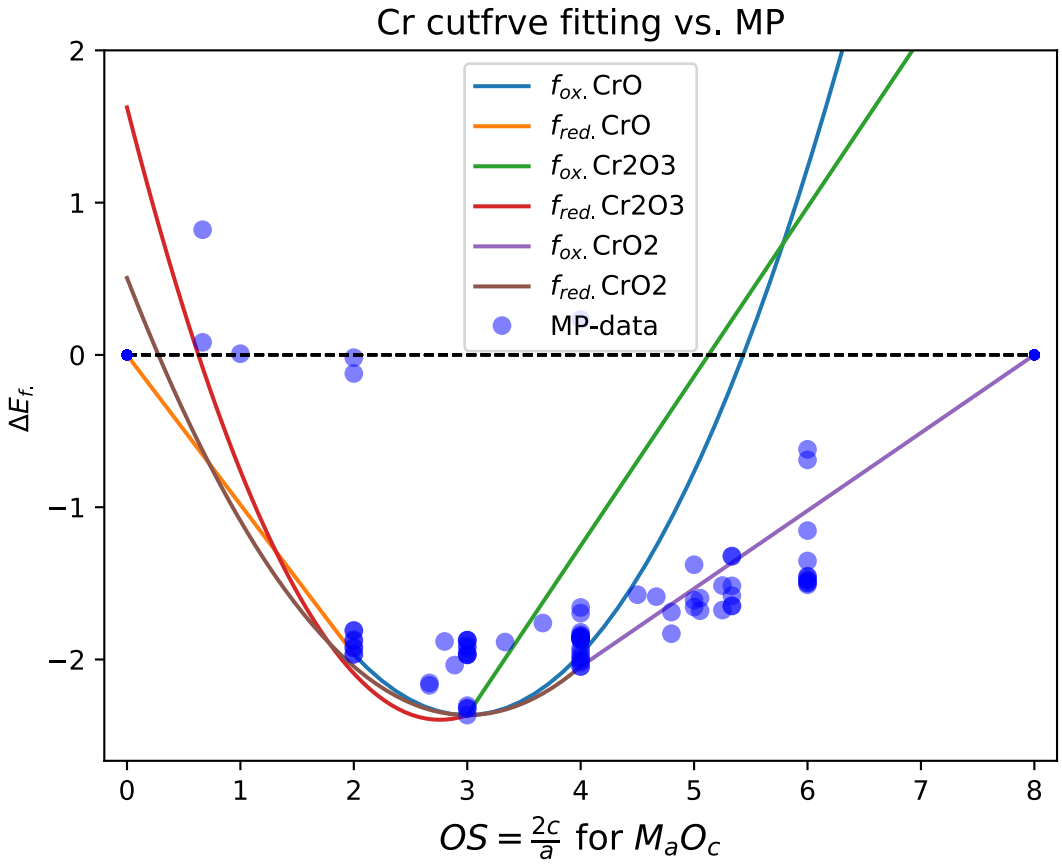

Br cutfrve fitting vs. MP
$f_{ox.}$ Br2O3
$f_{red.}$ Br2O3
$f_{ox.}$ BrO2
$f_{red.}$ BrO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

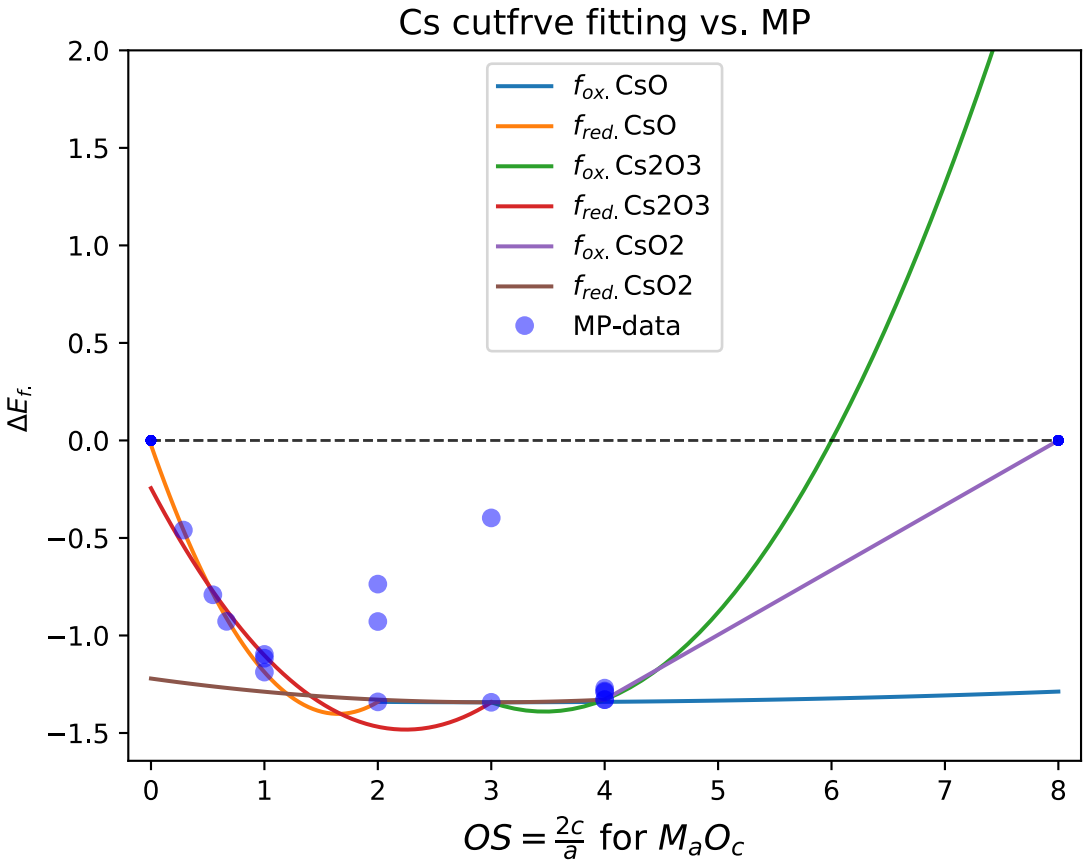

Ca cutfrve fitting vs. MP
$f_{ox.}$ CaO
$f_{red.}$ CaO
$f_{ox.}$ Ca2O3
$f_{red.}$ Ca2O3
$f_{ox.}$ CaO2
$f_{red.}$ CaO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

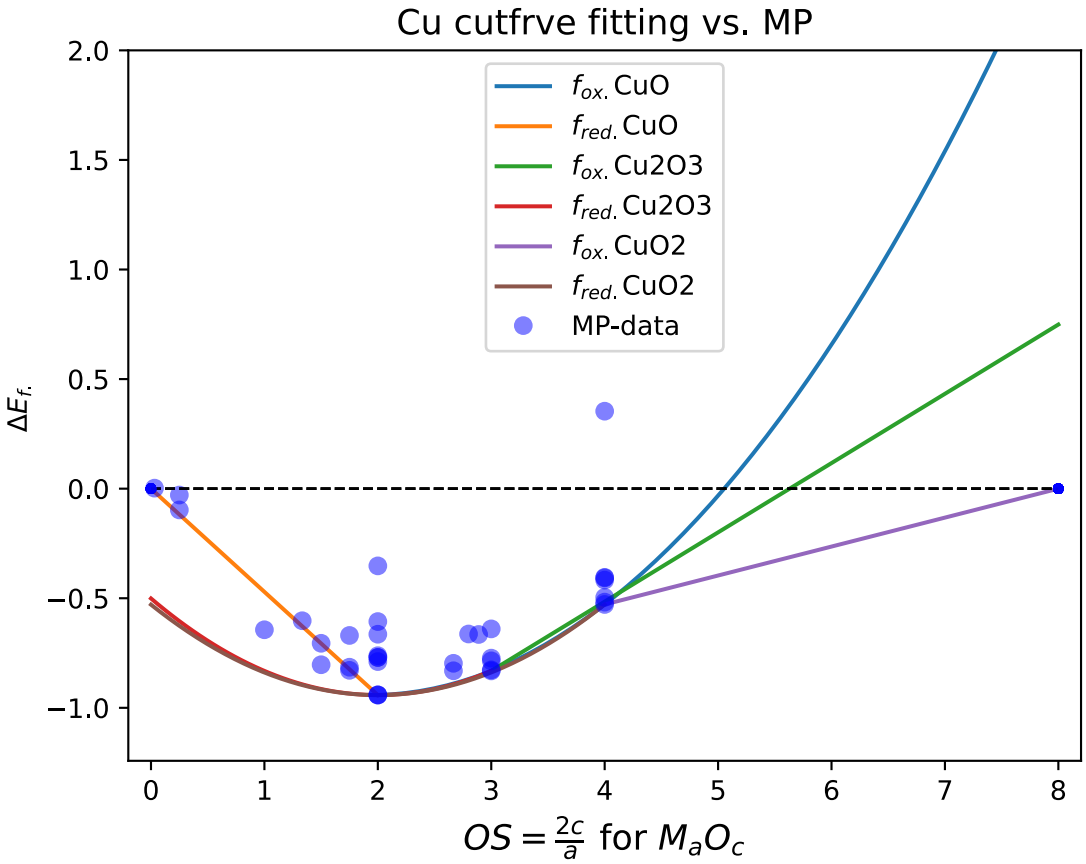

Cd cutfrve fitting vs. MP
$f_{ox.}$ CdO
$f_{red.}$ CdO
$f_{ox.}$ CdO2
$f_{red.}$ CdO2
MP-data
ΔE_f.
$OS = \frac{2c}{a}$ for M_aO_c

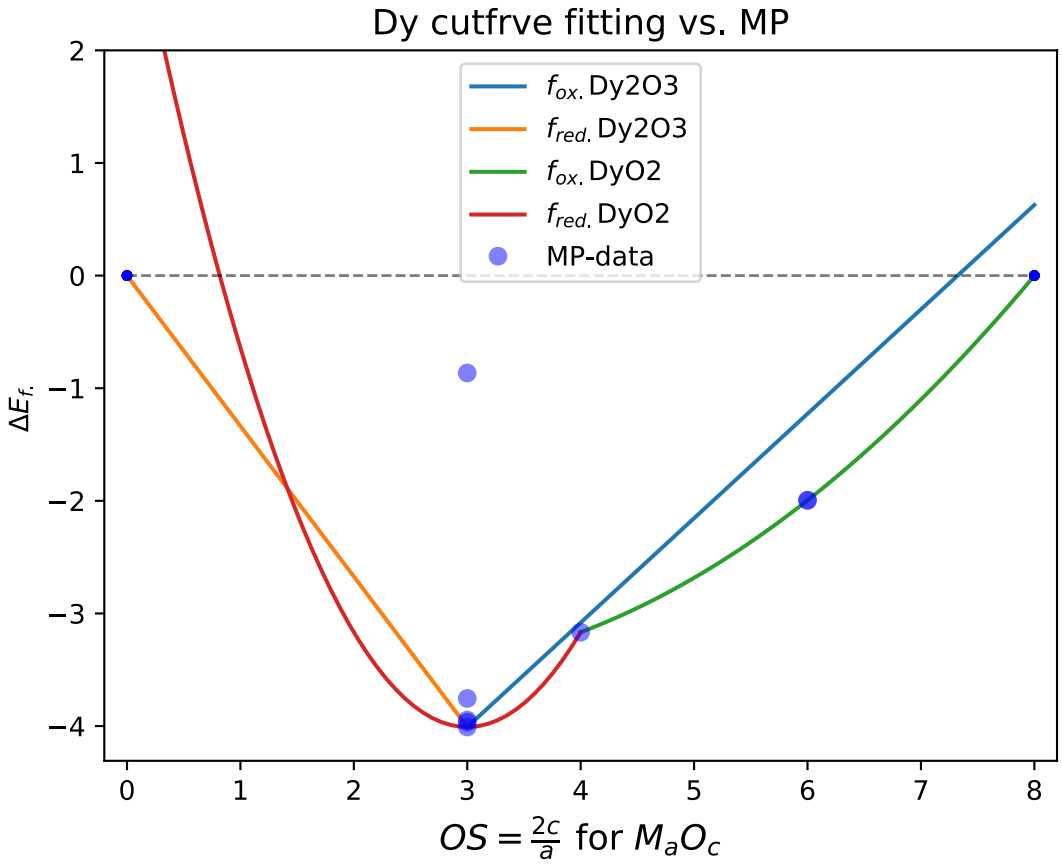

Ce cutfrve fitting vs. MP
$f_{ox.}$ CeO
$f_{red.}$ CeO
$f_{ox.}$ Ce2O3
$f_{red.}$ Ce2O3
$f_{ox.}$ CeO2
$f_{red.}$ CeO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

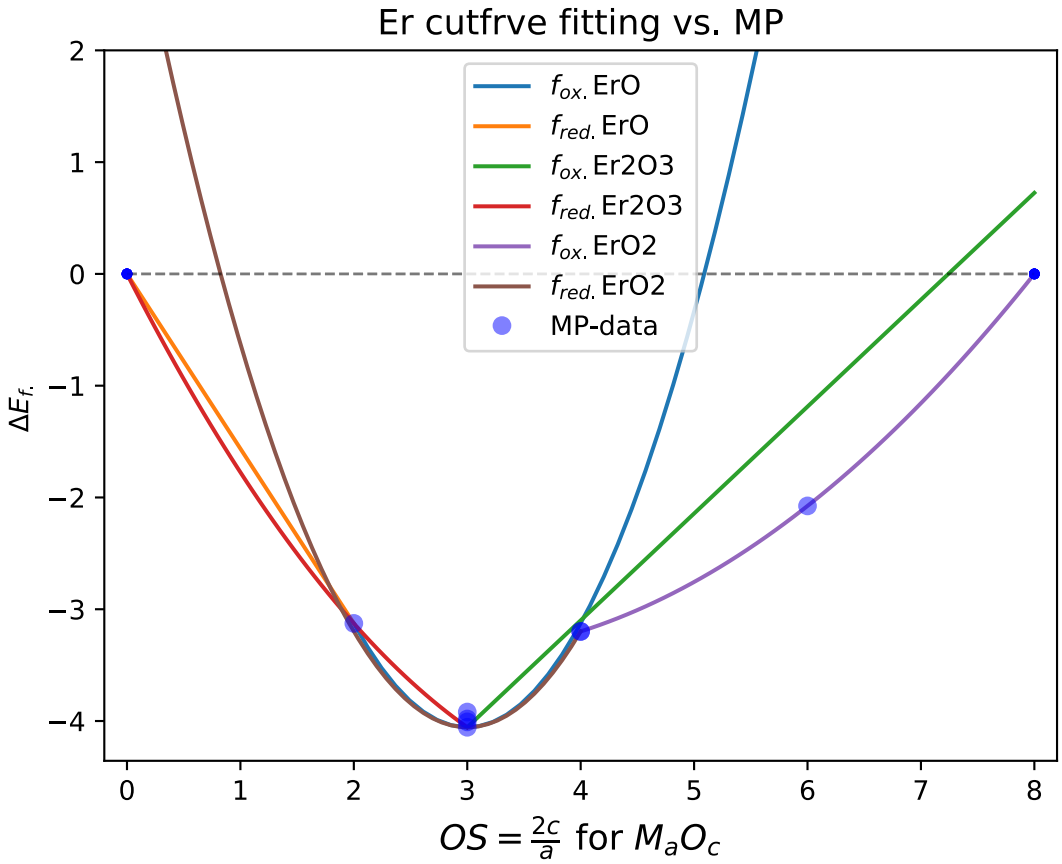

Co cutfrve fitting vs. MP
$f_{ox.}$ CoO
$f_{red.}$ CoO
$f_{ox.}$ Co2O3
$f_{red.}$ Co2O3
$f_{ox.}$ CoO2
$f_{red.}$ CoO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

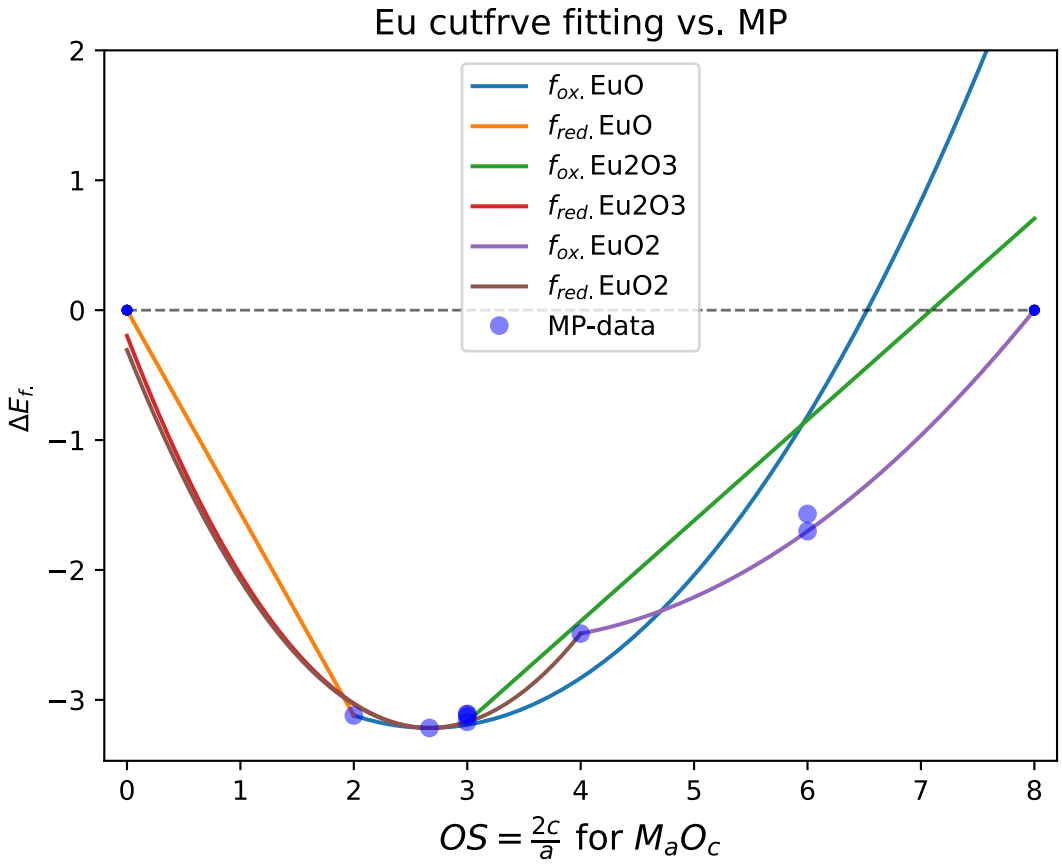

Cr cutfrve fitting vs. MP
$f_{ox.}$ CrO
$f_{red.}$ CrO
$f_{ox.}$ Cr2O3
$f_{red.}$ Cr2O3
$f_{ox.}$ CrO2
$f_{red.}$ CrO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

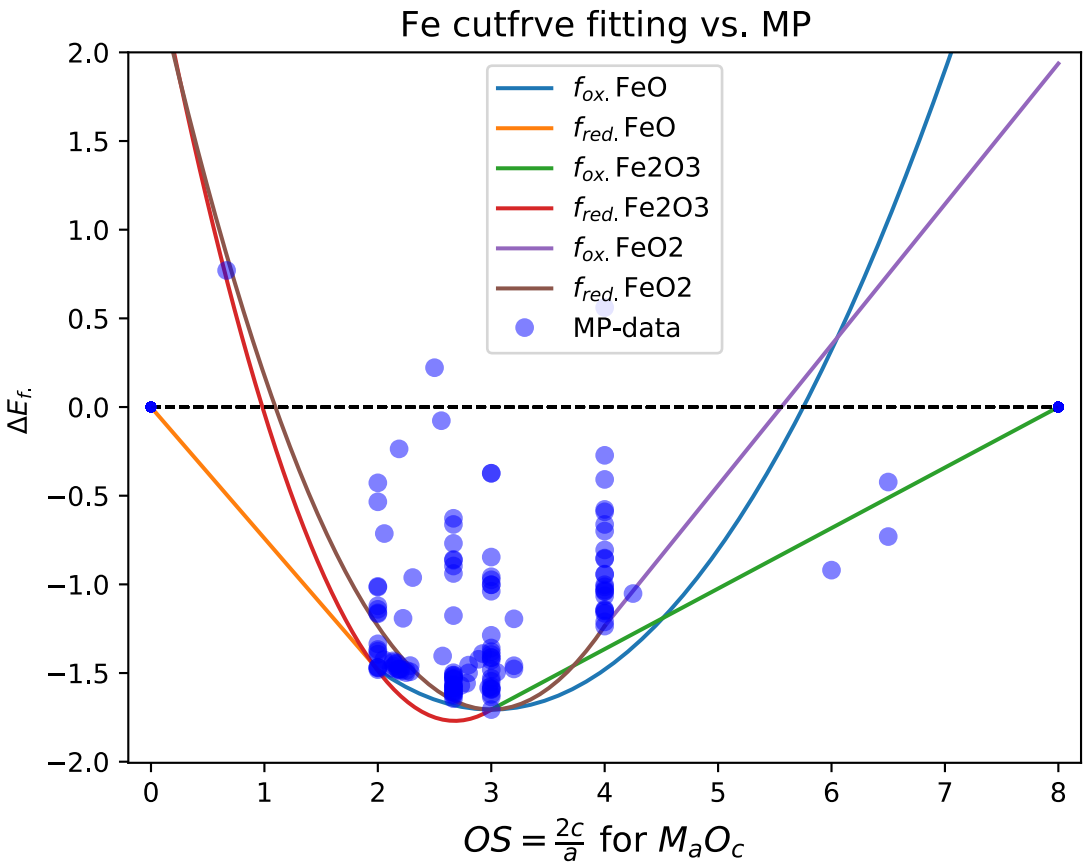

Cs cutfrve fitting vs. MP
$f_{ox.}$ CsO
$f_{red.}$ CsO
$f_{ox.}$ Cs2O3
$f_{red.}$ Cs2O3
$f_{ox.}$ CsO2
$f_{red.}$ CsO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

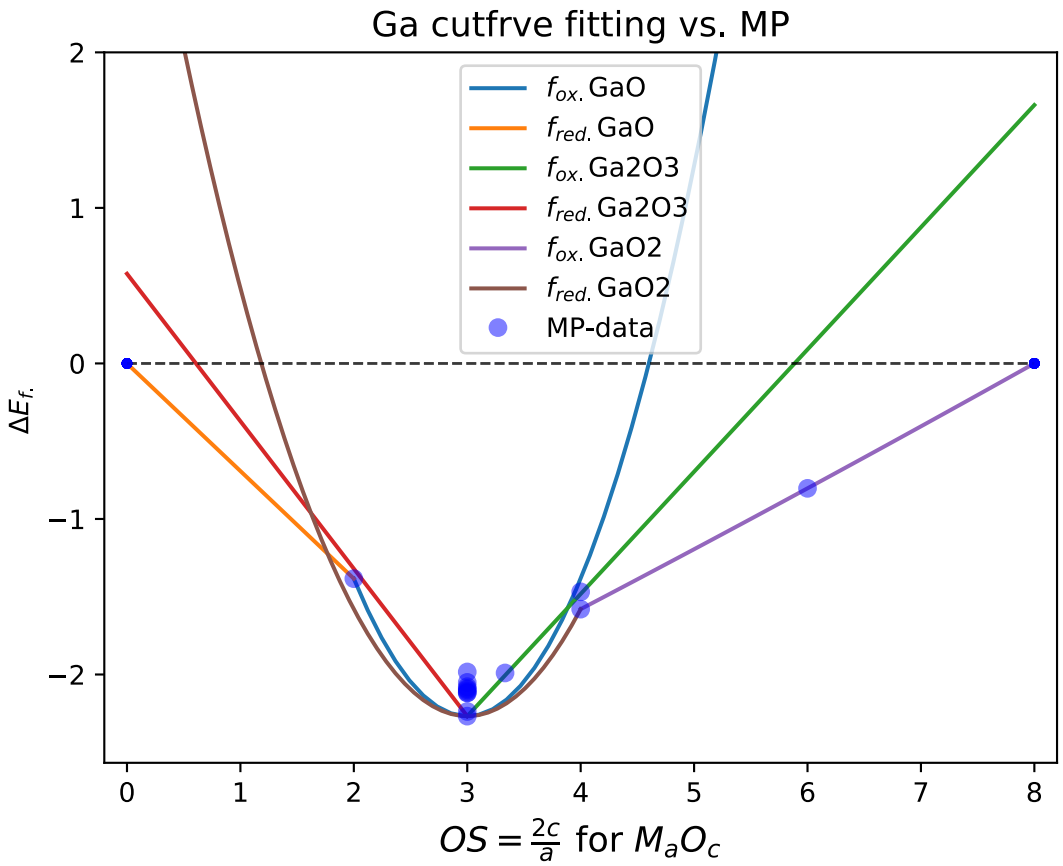

Cu cutfrve fitting vs. MP
$f_{ox.}$ CuO
$f_{red.}$ CuO
$f_{ox.}$ Cu2O3
$f_{red.}$ Cu2O3
$f_{ox.}$ CuO2
$f_{red.}$ CuO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

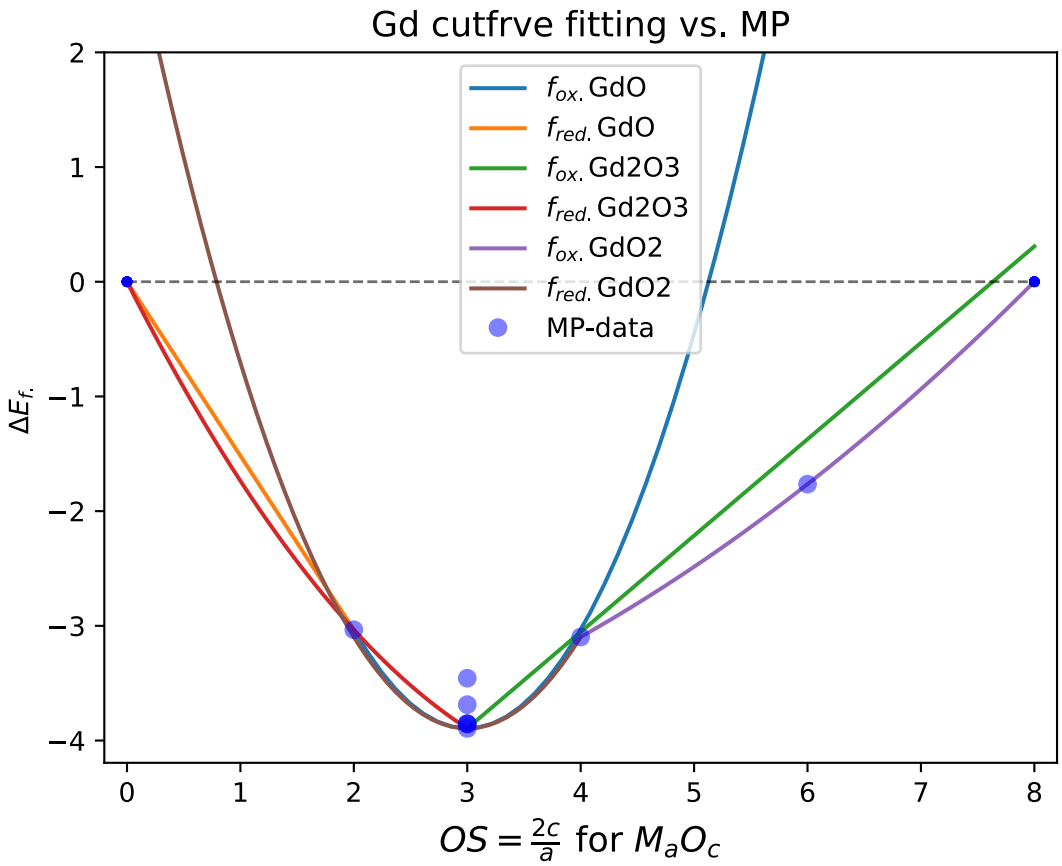

Dy cutfrve fitting vs. MP
$f_{ox.}$ Dy2O3
$f_{red.}$ Dy2O3
$f_{ox.}$ DyO2
$f_{red.}$ DyO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

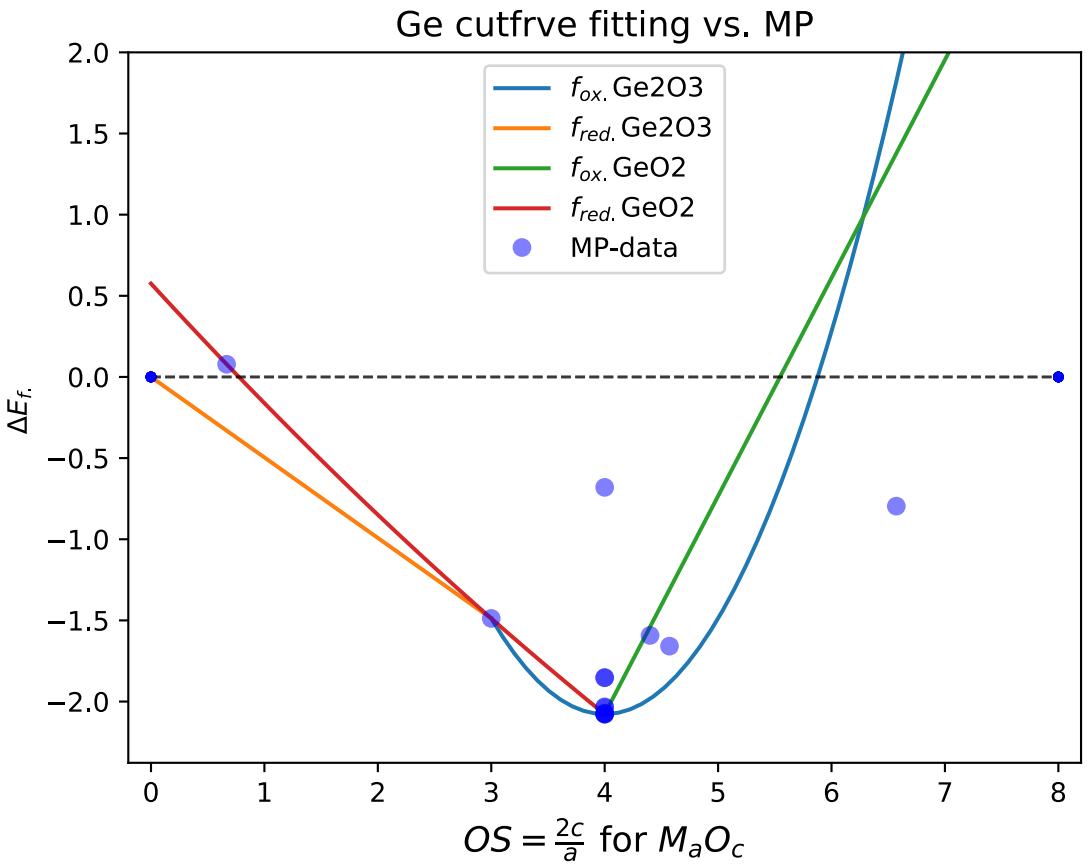

Er cutfrve fitting vs. MP
$f_{ox.}$ ErO
$f_{red.}$ ErO
$f_{ox.}$ Er2O3
$f_{red.}$ Er2O3
$f_{ox.}$ ErO2
$f_{red.}$ ErO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

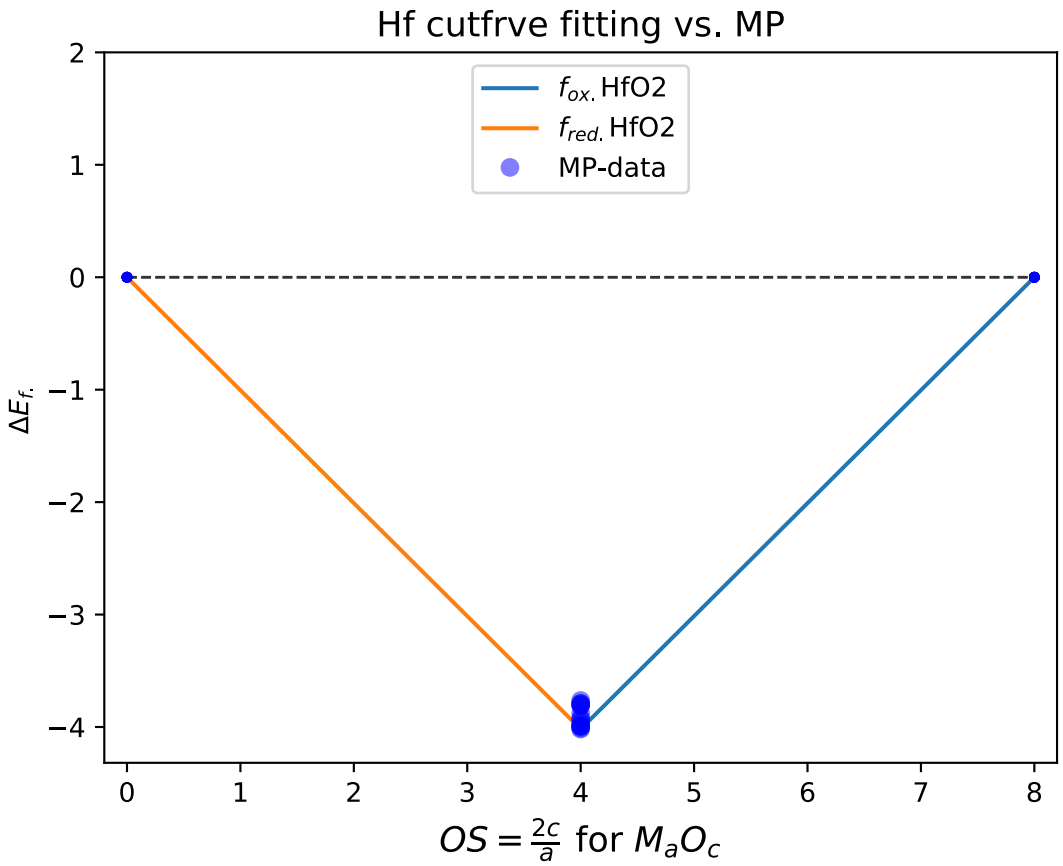

Eu cutfrve fitting vs. MP
$f_{ox.}$ EuO
$f_{red.}$ EuO
$f_{ox.}$ Eu2O3
$f_{red.}$ Eu2O3
$f_{ox.}$ EuO2
$f_{red.}$ EuO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

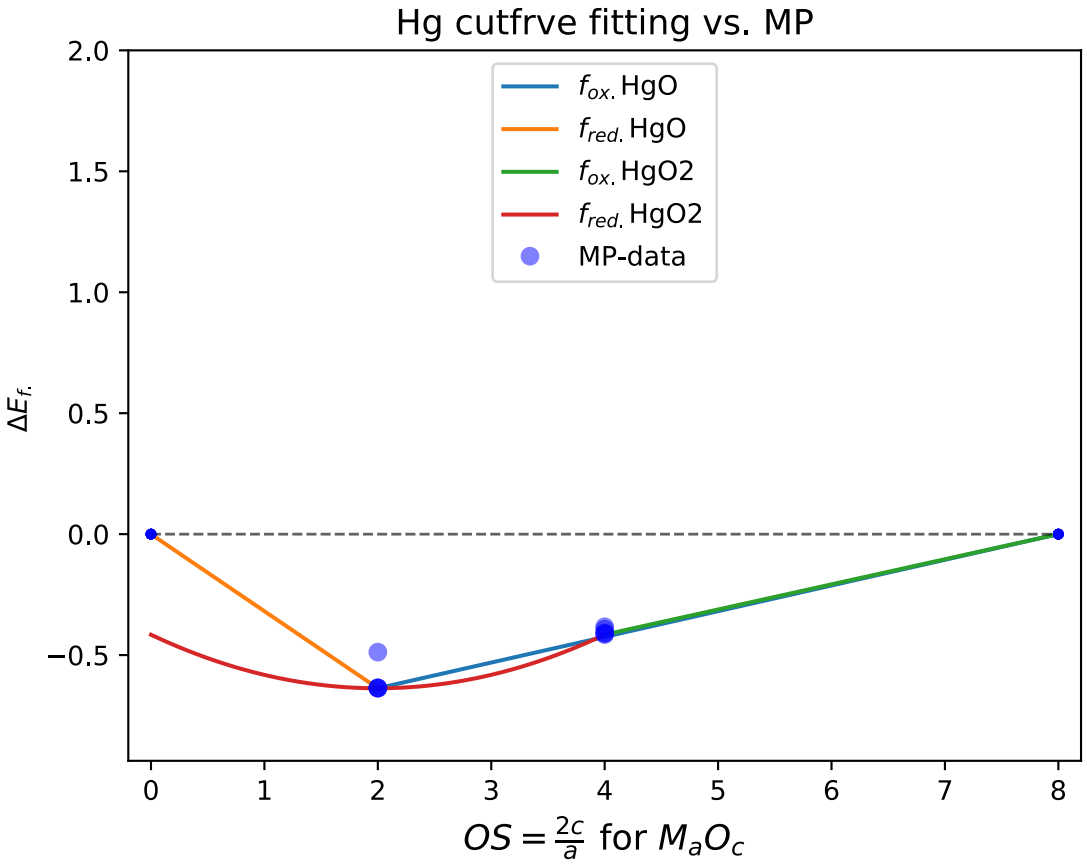

Fe cutfrve fitting vs. MP
$f_{ox.}$ FeO
$f_{red.}$ FeO
$f_{ox.}$ Fe2O3
$f_{red.}$ Fe2O3
$f_{ox.}$ FeO2
$f_{red.}$ FeO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

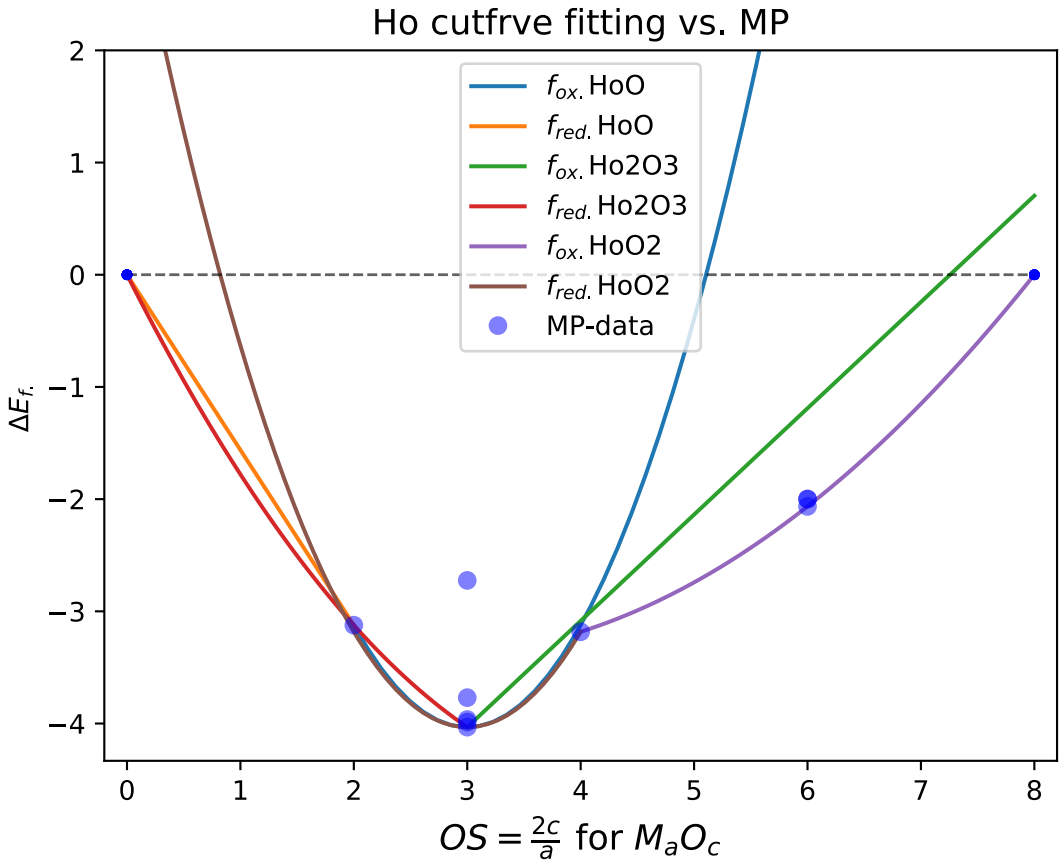

Ga cutfrve fitting vs. MP
$f_{ox.}$ GaO
$f_{red.}$ GaO
$f_{ox.}$ Ga2O3
$f_{red.}$ Ga2O3
$f_{ox.}$ GaO2
$f_{red.}$ GaO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

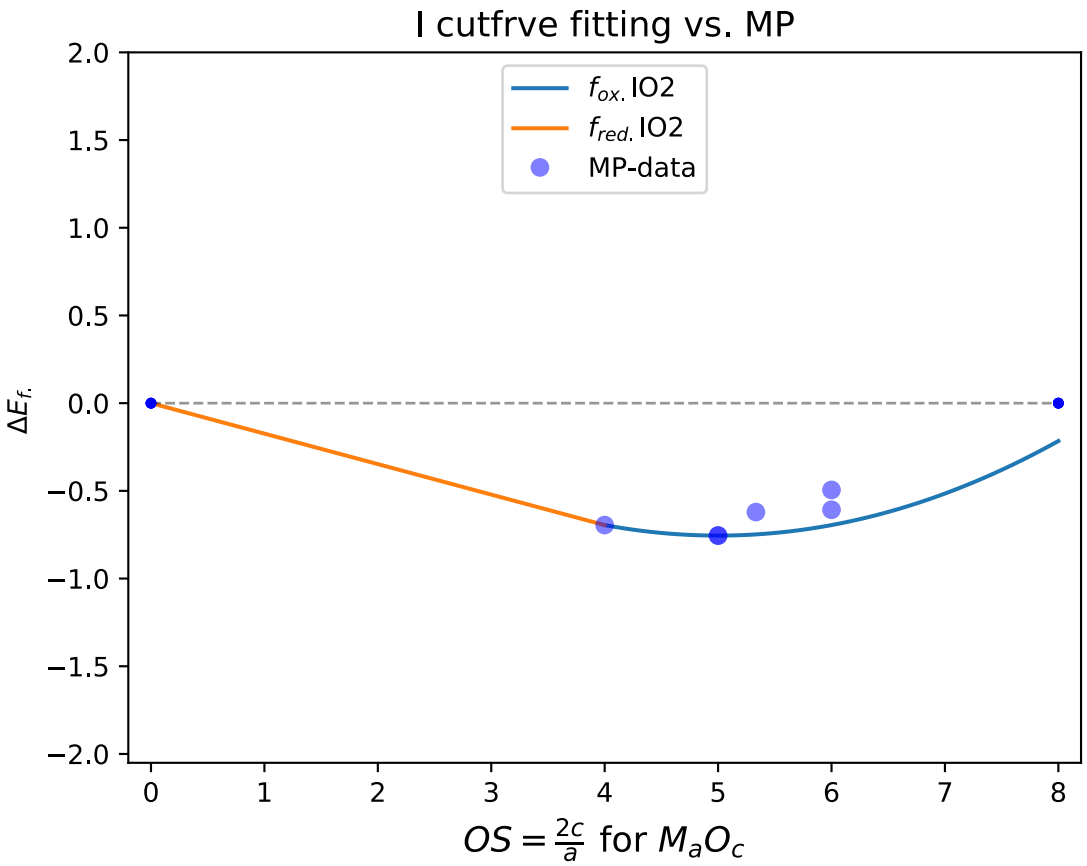

Gd cutfrve fitting vs. MP
$f_{ox.}$ GdO
$f_{red.}$ GdO
$f_{ox.}$ Gd2O3
$f_{red.}$ Gd2O3
$f_{ox.}$ GdO2
$f_{red.}$ GdO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

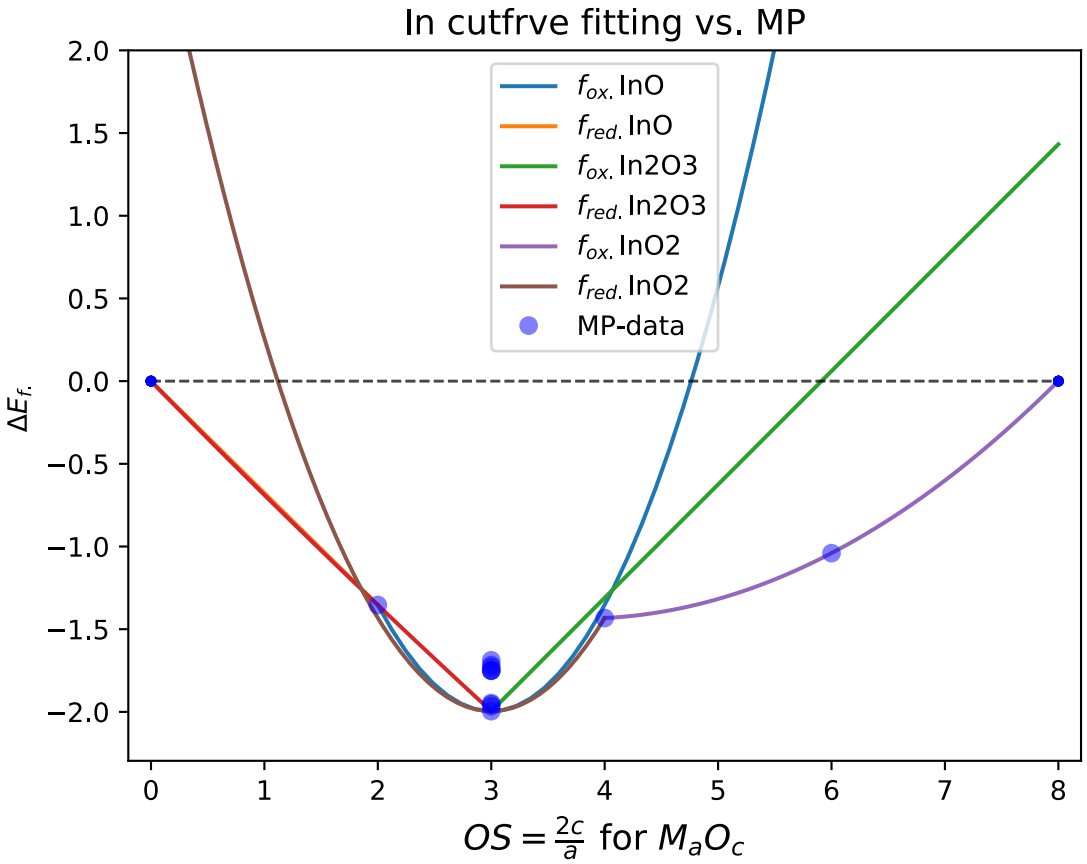

Ge cutfrve fitting vs. MP
$f_{ox.}$ Ge2O3
$f_{red.}$ Ge2O3
$f_{ox.}$ GeO2
$f_{red.}$ GeO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

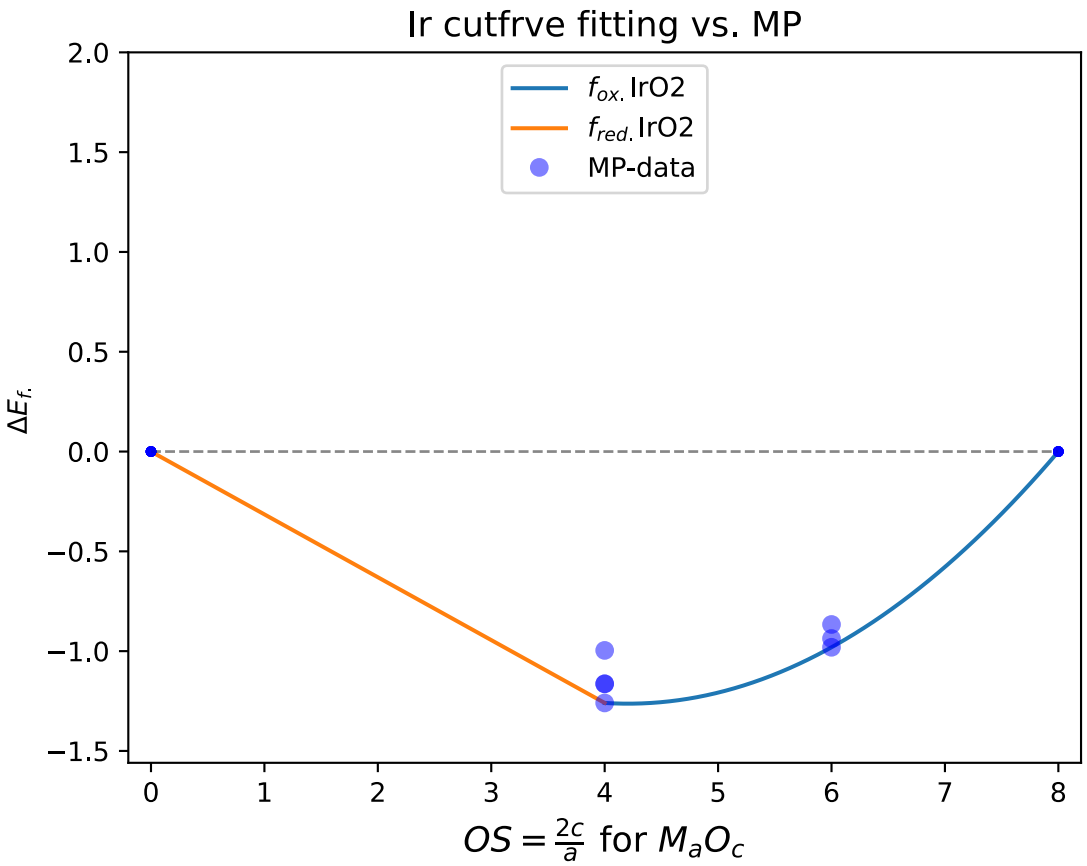

Hf cutfrve fitting vs. MP
$f_{ox.}$ HfO2
$f_{red.}$ HfO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c


Hg cutfrve fitting vs. MP
$f_{ox.}$ HgO
$f_{red.}$ HgO
$f_{ox.}$ HgO2
$f_{red.}$ HgO2
MP-data
$\Delta E_{f.}$
2.0
1.5
1.0
0.5
0.0
−0.5
0
1
2
3
4
5
6
7
8
$OS = \frac{2c}{a}$ for M_aO_c


Ho cutfrve fitting vs. MP
$f_{ox.}$ HoO
$f_{red.}$ HoO
$f_{ox.}$ Ho2O3
$f_{red.}$ Ho2O3
$f_{ox.}$ HoO2
$f_{red.}$ HoO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c


I cutfrve fitting vs. MP
$f_{ox.}$ IO2
$f_{red.}$ IO2
MP-data
ΔE_f.
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
0
1
2
3
4
5
6
7
8
$OS = \frac{2c}{a}$ for M_aO_c


In cutfrve fitting vs. MP
$f_{ox.}$ InO
$f_{red.}$ InO
$f_{ox.}$ In2O3
$f_{red.}$ In2O3
$f_{ox.}$ InO2
$f_{red.}$ InO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c


Ir cutfrve fitting vs. MP
$f_{ox.}$ IrO2
$f_{red.}$ IrO2
MP-data
ΔE_f.
2.0
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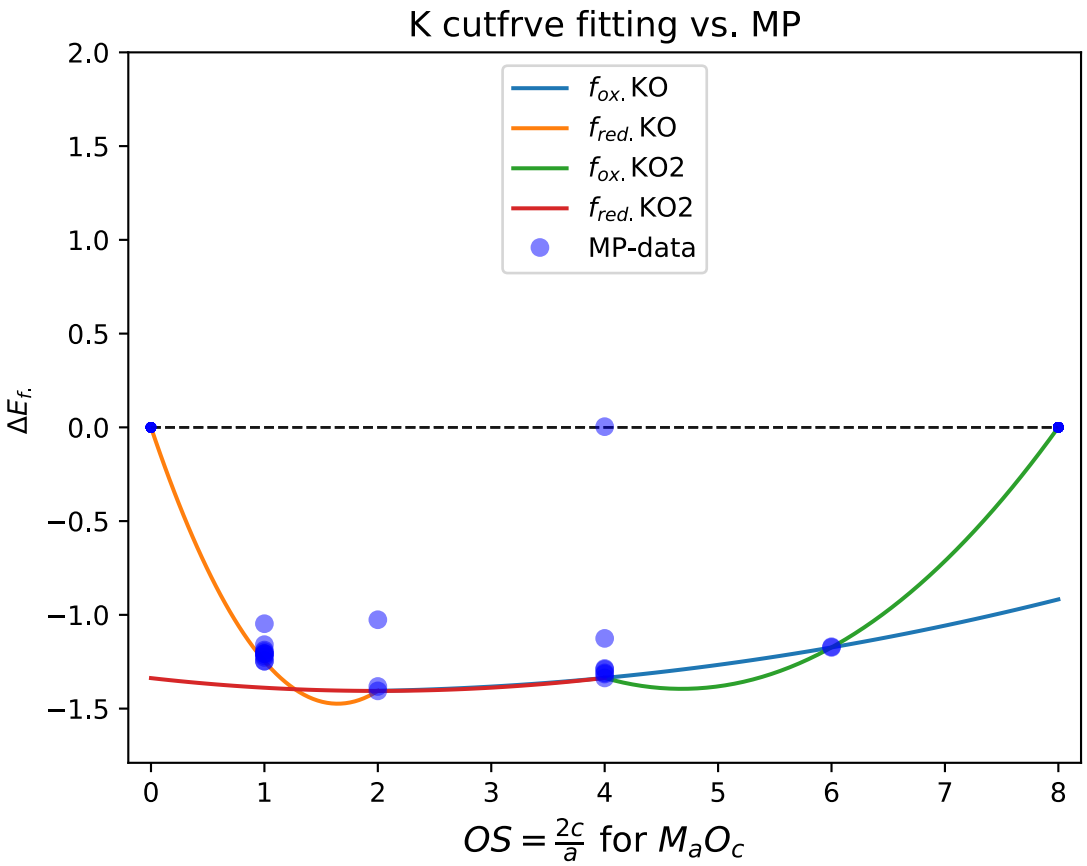
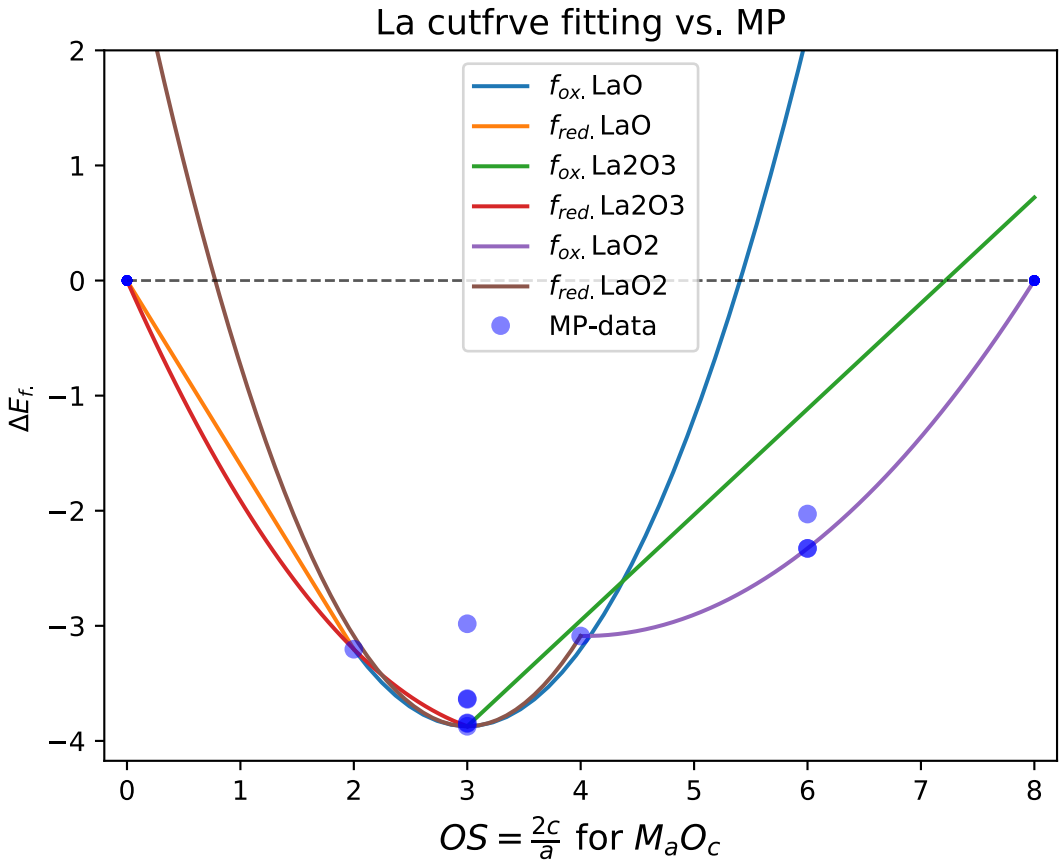
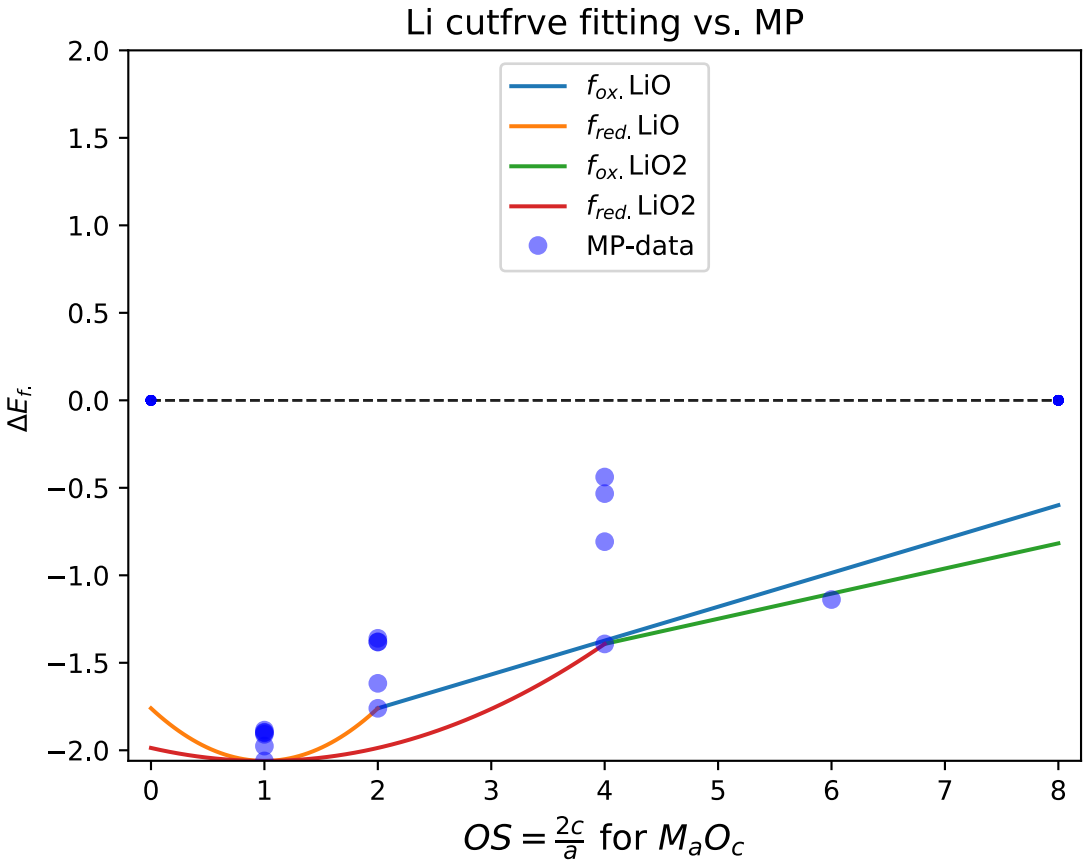
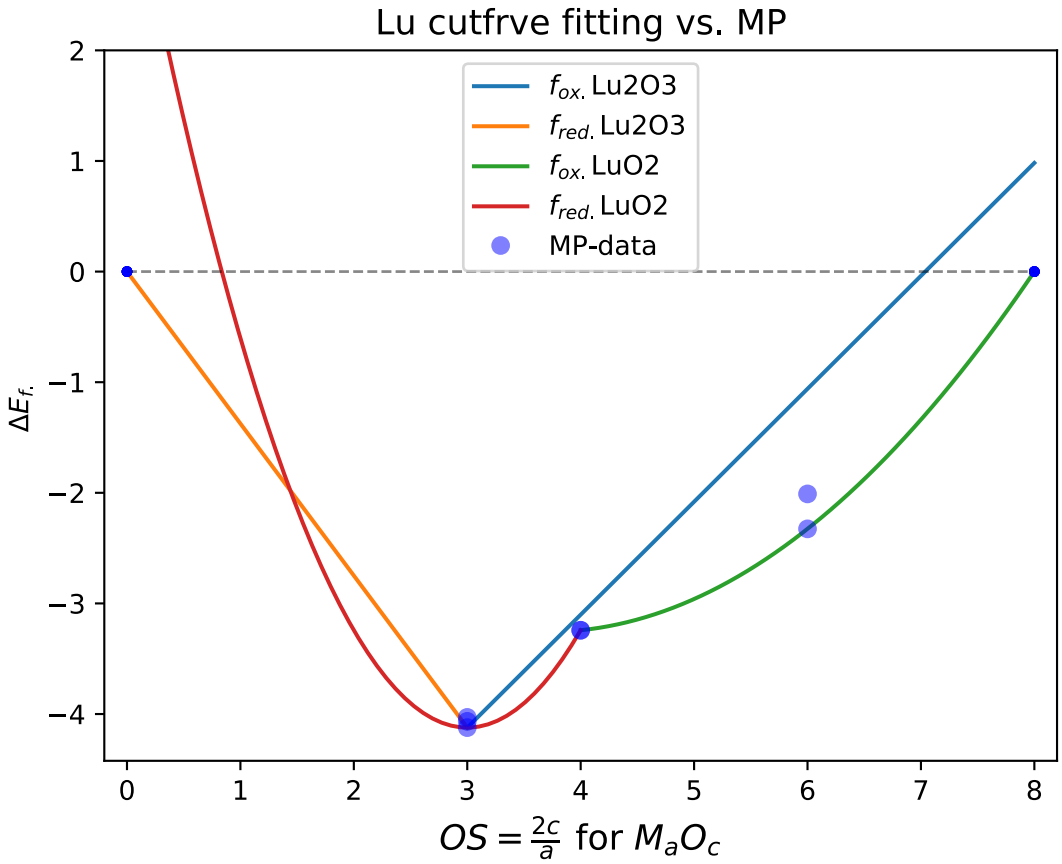
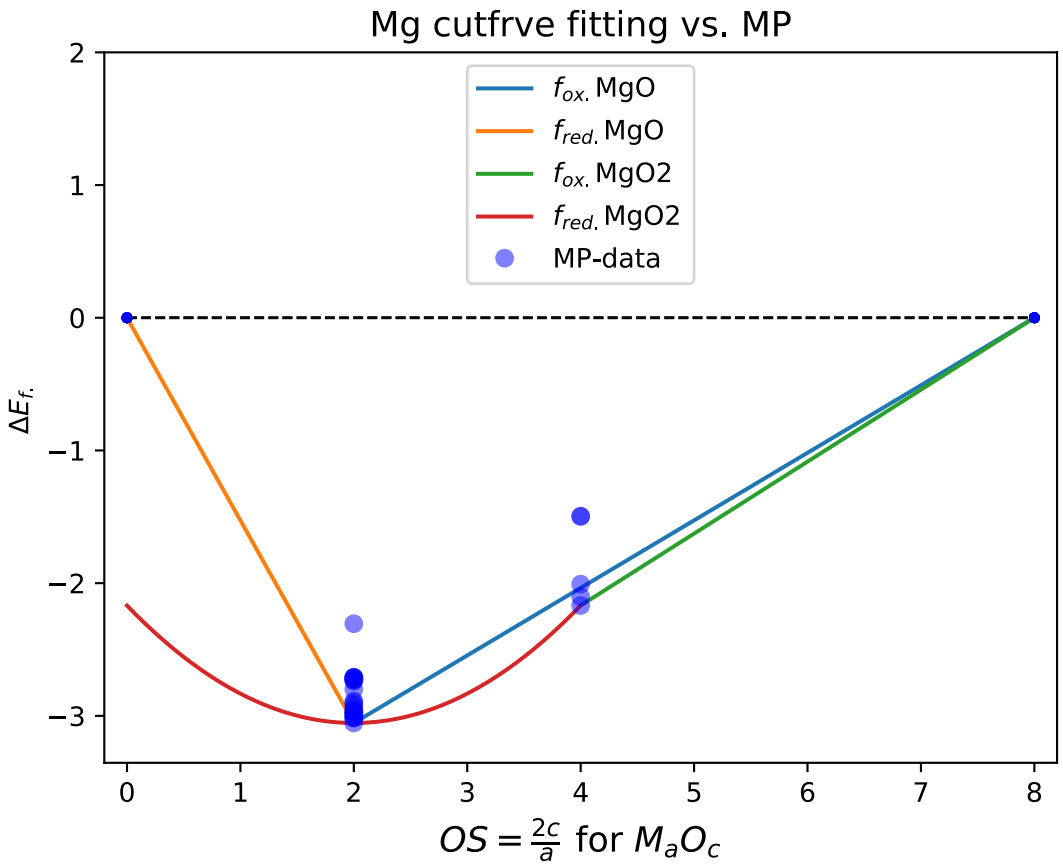
1.0
0.5
0.0
−0.5
−1.0
−1.5
0
1
2
3
4
5
6
7
8
$OS = \frac{2c}{a}$ for M_aO_c

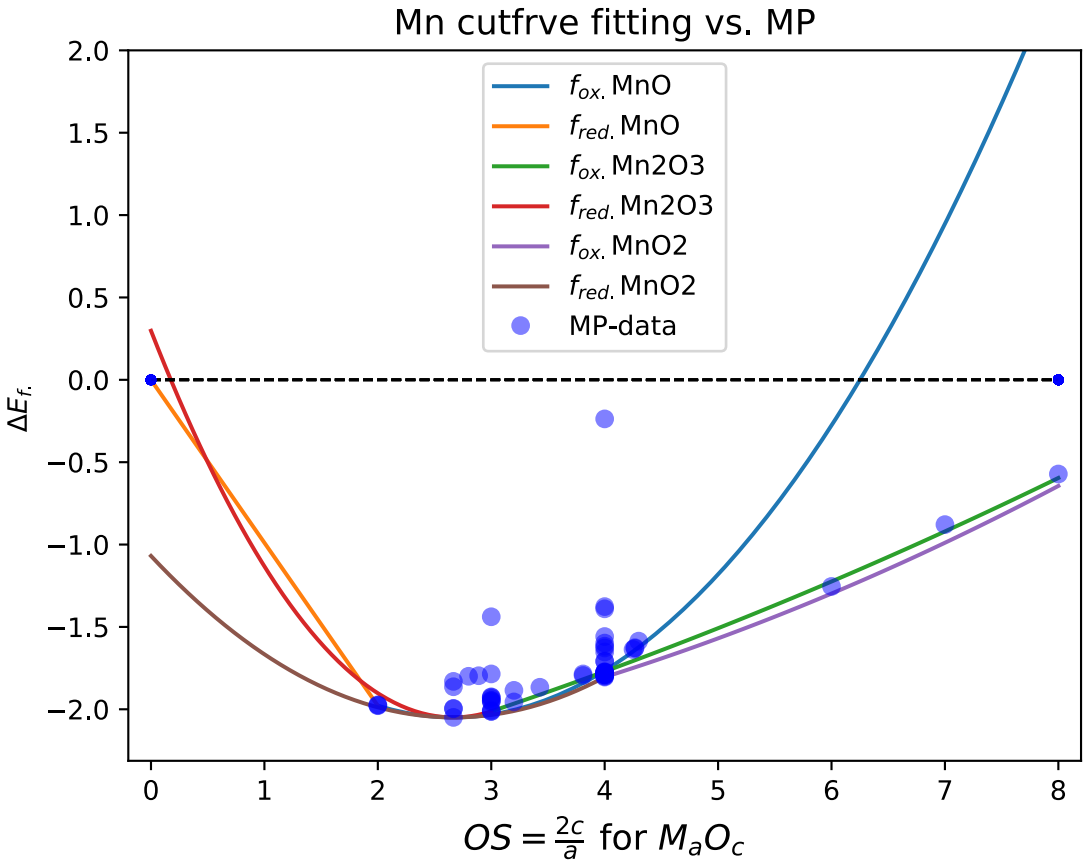

K cutfrve fitting vs. MP
$f_{ox.}$ KO
$f_{red.}$ KO
$f_{ox.}$ KO2
$f_{red.}$ KO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

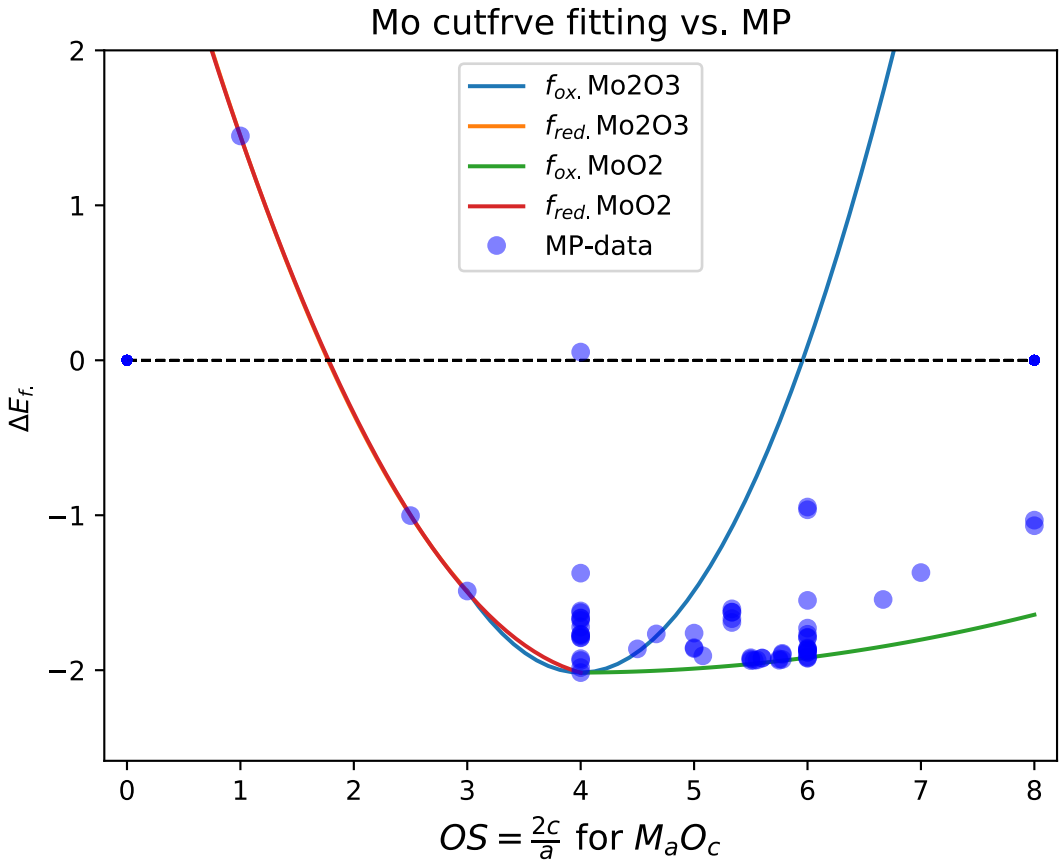

La cutfrve fitting vs. MP
$f_{ox.}$ LaO
$f_{red.}$ LaO
$f_{ox.}$ La2O3
$f_{red.}$ La2O3
$f_{ox.}$ LaO2
$f_{red.}$ LaO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

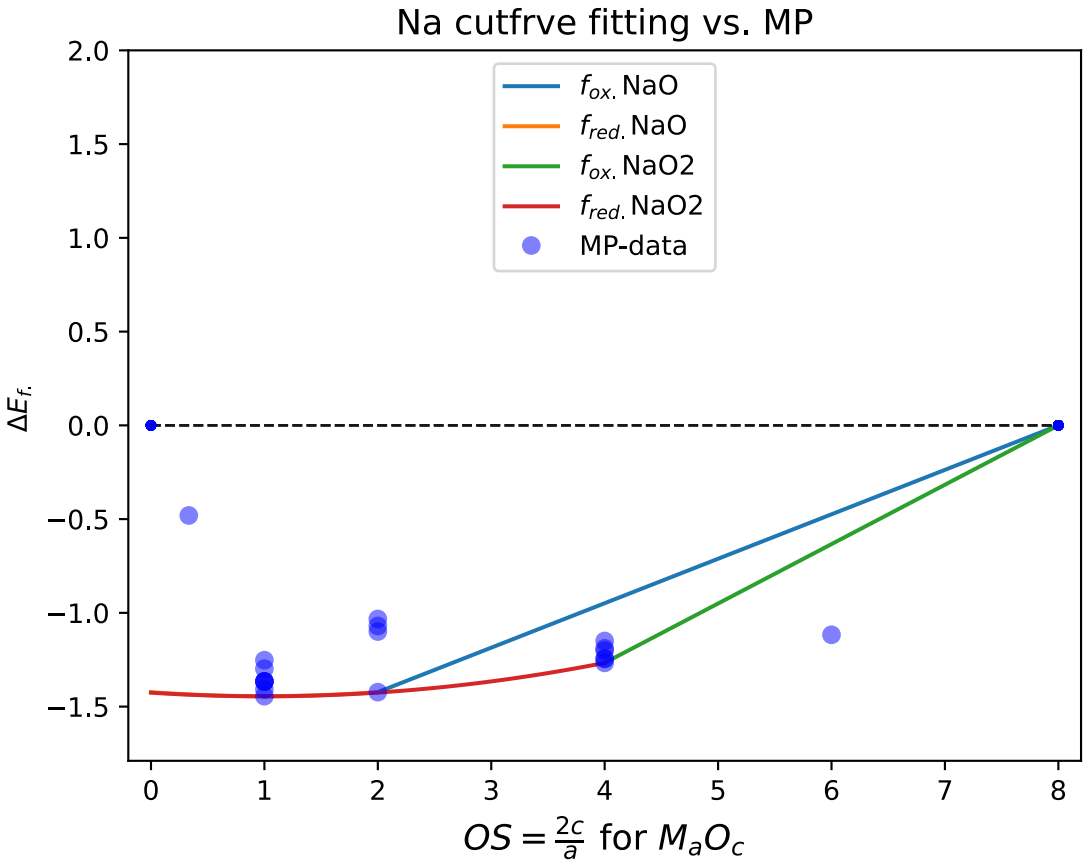

Li cutfrve fitting vs. MP
$f_{ox.}$ LiO
$f_{red.}$ LiO
$f_{ox.}$ LiO2
$f_{red.}$ LiO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

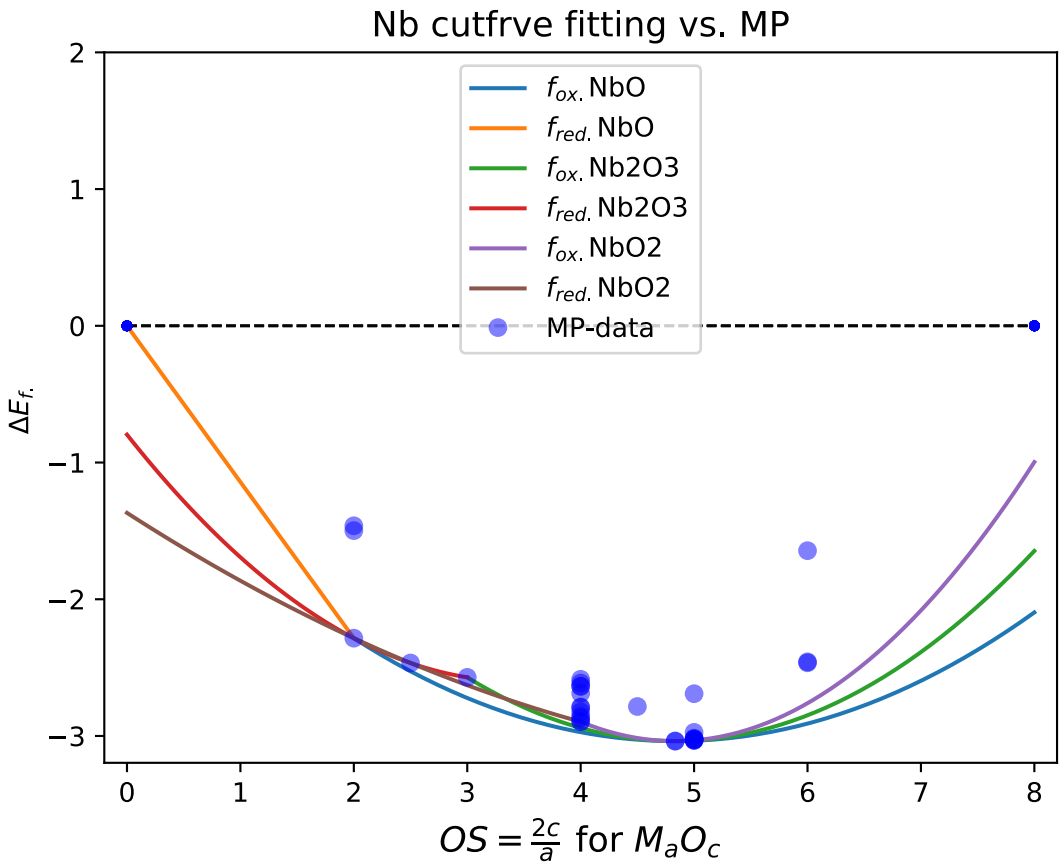

Lu cutfrve fitting vs. MP
$f_{ox.}$ Lu2O3
$f_{red.}$ Lu2O3
$f_{ox.}$ LuO2
$f_{red.}$ LuO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

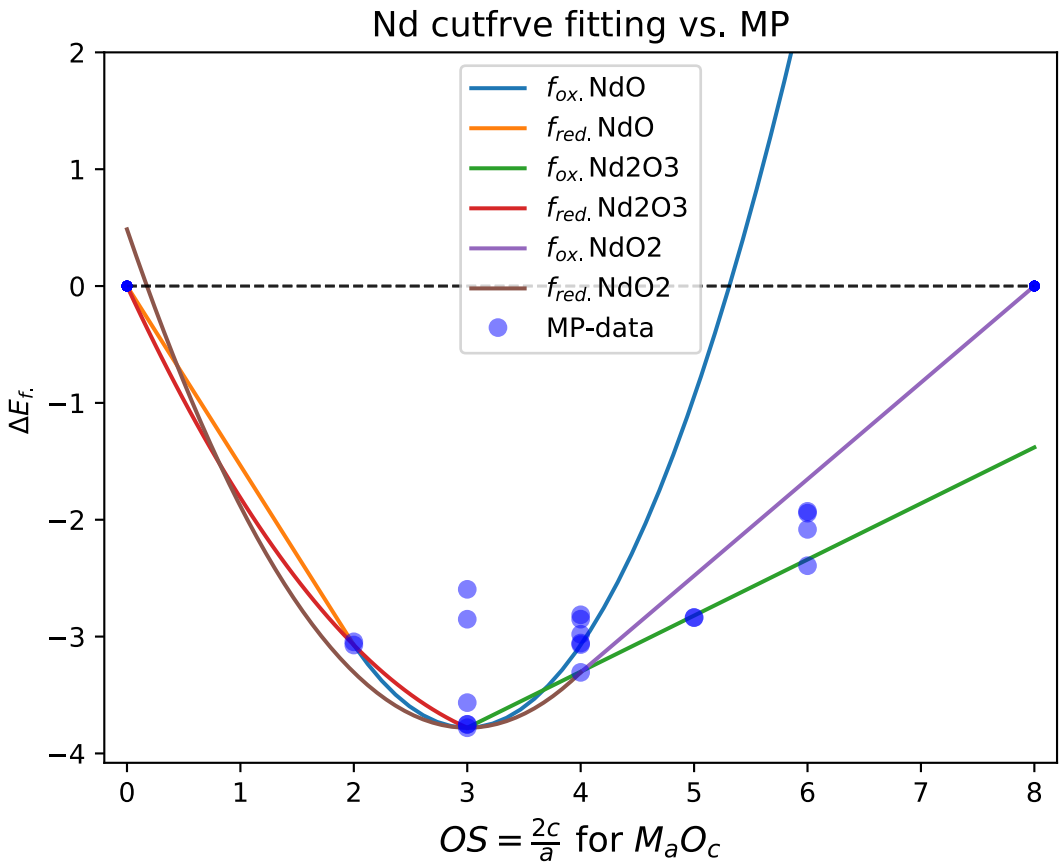

Mg cutfrve fitting vs. MP
$f_{ox.}$ MgO
$f_{red.}$ MgO
$f_{ox.}$ MgO2
$f_{red.}$ MgO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

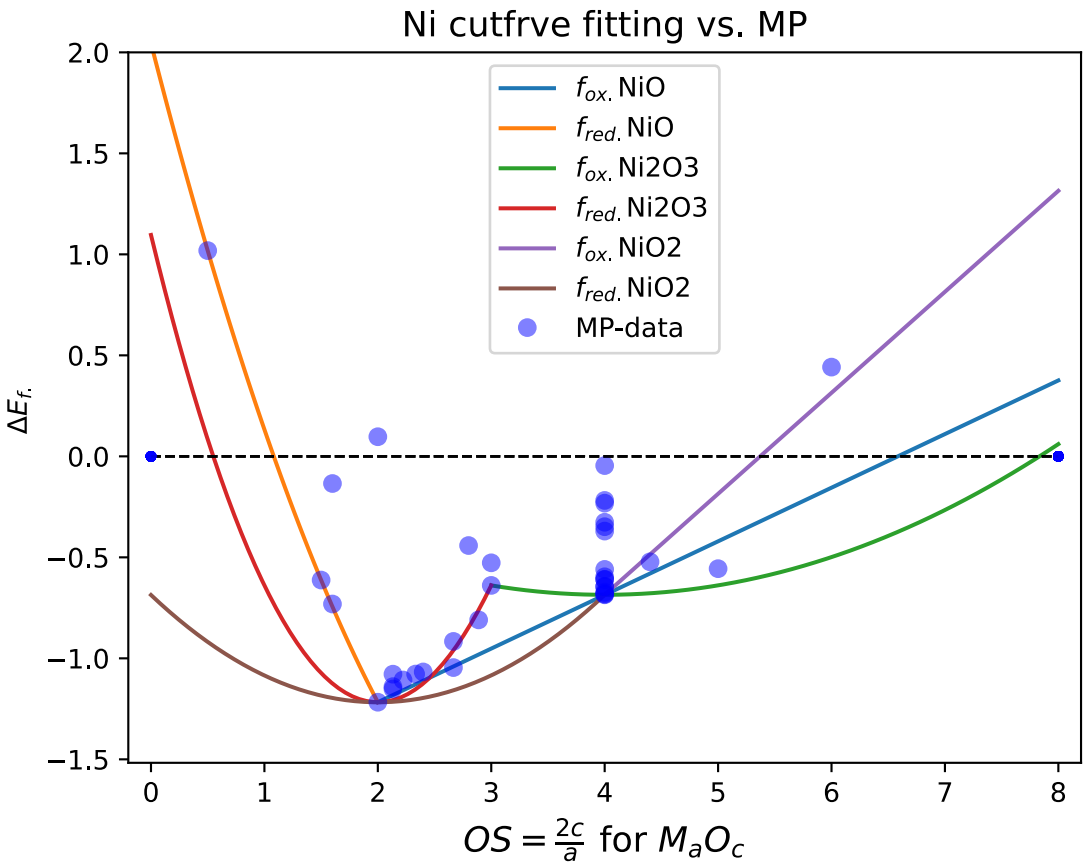

Mn cutfrve fitting vs. MP
$f_{ox.}$ MnO
$f_{red.}$ MnO
$f_{ox.}$ Mn2O3
$f_{red.}$ Mn2O3
$f_{ox.}$ MnO2
$f_{red.}$ MnO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

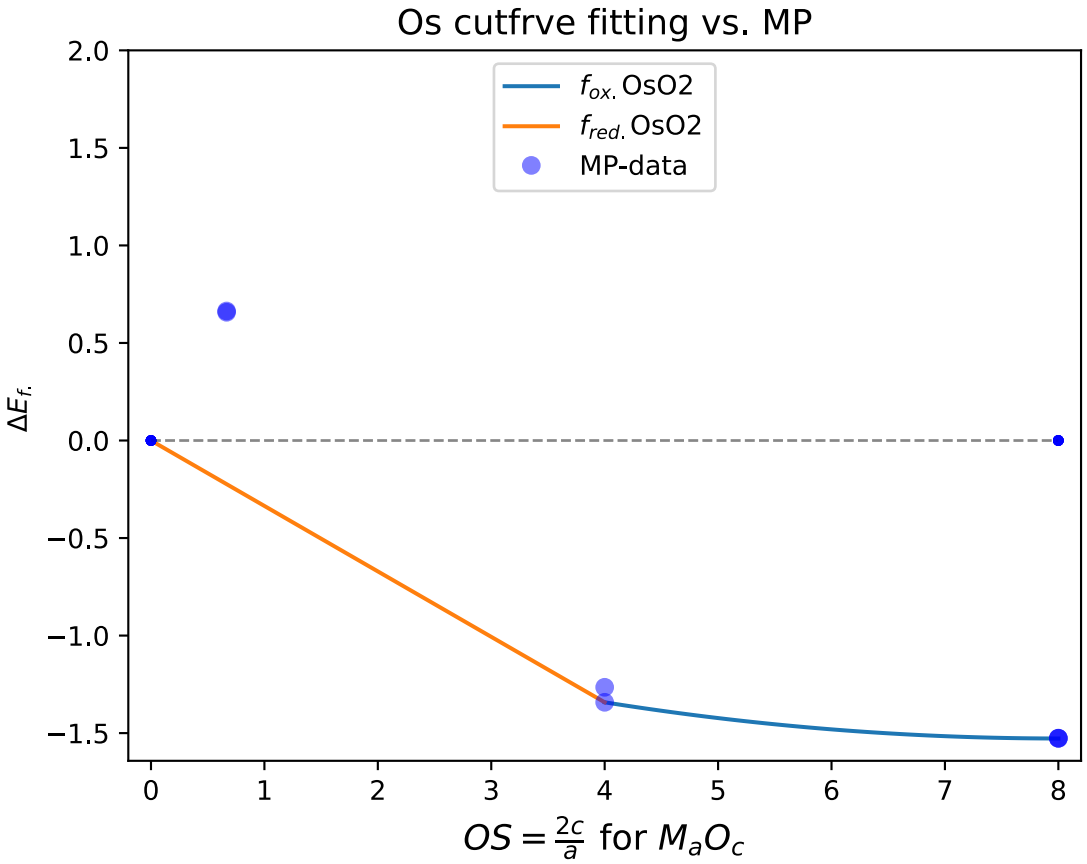

Mo cutfrve fitting vs. MP
$f_{ox.}$ Mo2O3
$f_{red.}$ Mo2O3
$f_{ox.}$ MoO2
$f_{red.}$ MoO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

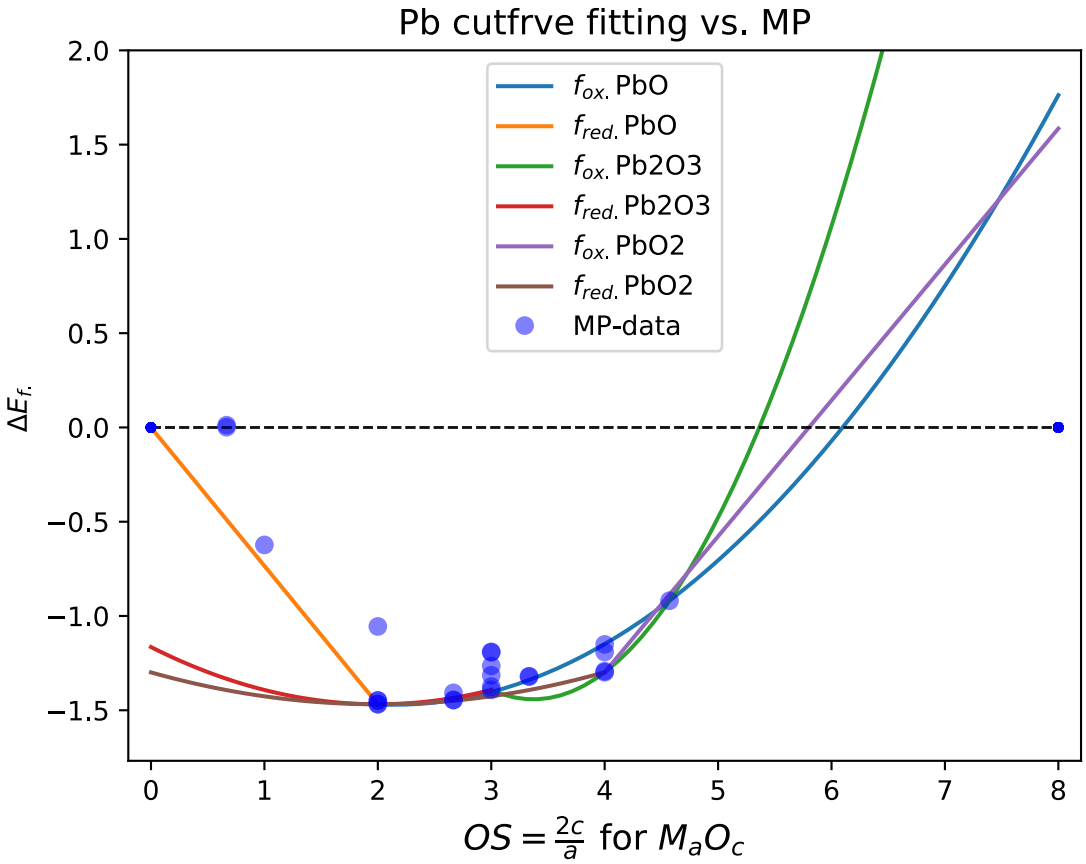

Na cutfrve fitting vs. MP
$f_{ox.}$ NaO
$f_{red.}$ NaO
$f_{ox.}$ NaO2
$f_{red.}$ NaO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

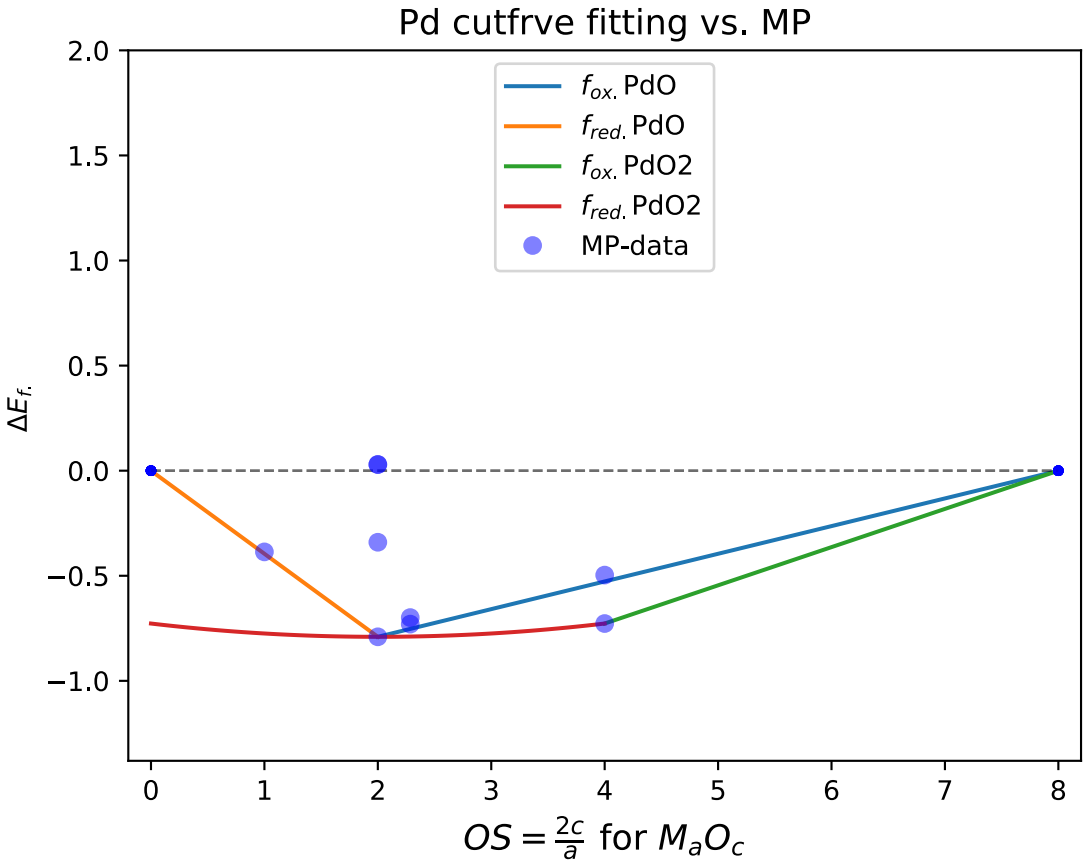

Nb cutfrve fitting vs. MP
$f_{ox.}$ NbO
$f_{red.}$ NbO
$f_{ox.}$ Nb2O3
$f_{red.}$ Nb2O3
$f_{ox.}$ NbO2
$f_{red.}$ NbO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

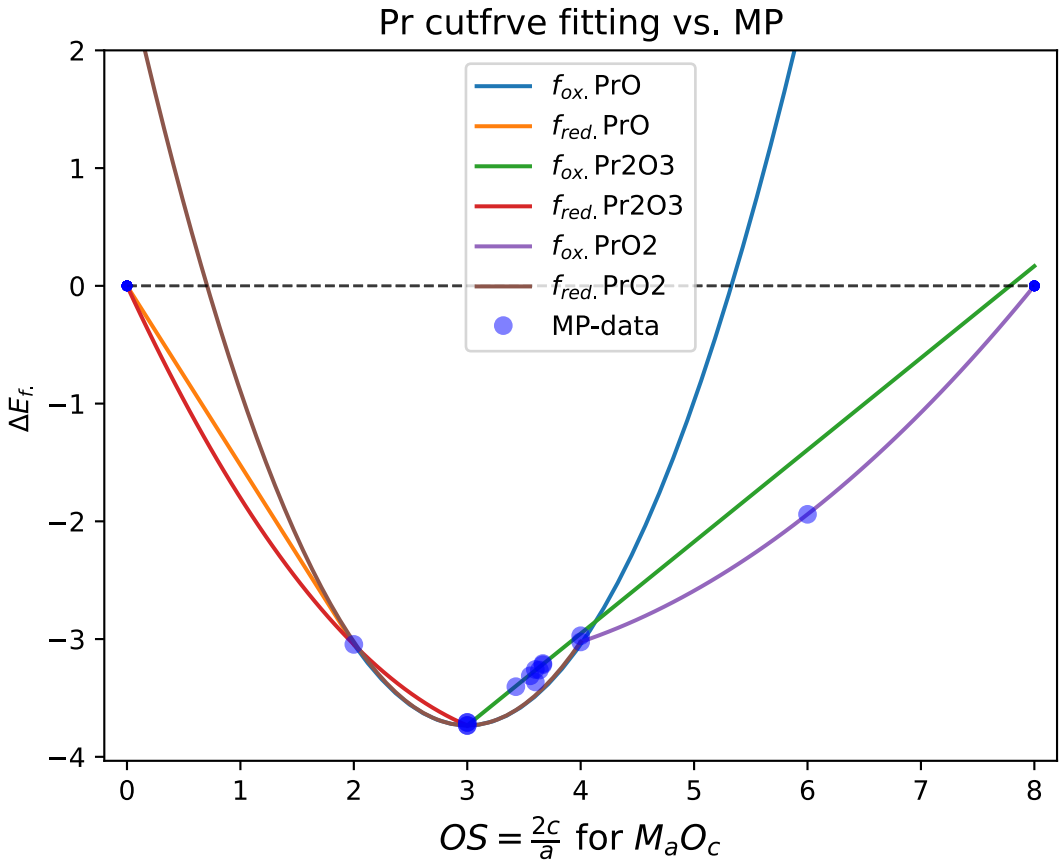

Nd cutfrve fitting vs. MP
$f_{ox.}$ NdO
$f_{red.}$ NdO
$f_{ox.}$ Nd2O3
$f_{red.}$ Nd2O3
$f_{ox.}$ NdO2
$f_{red.}$ NdO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

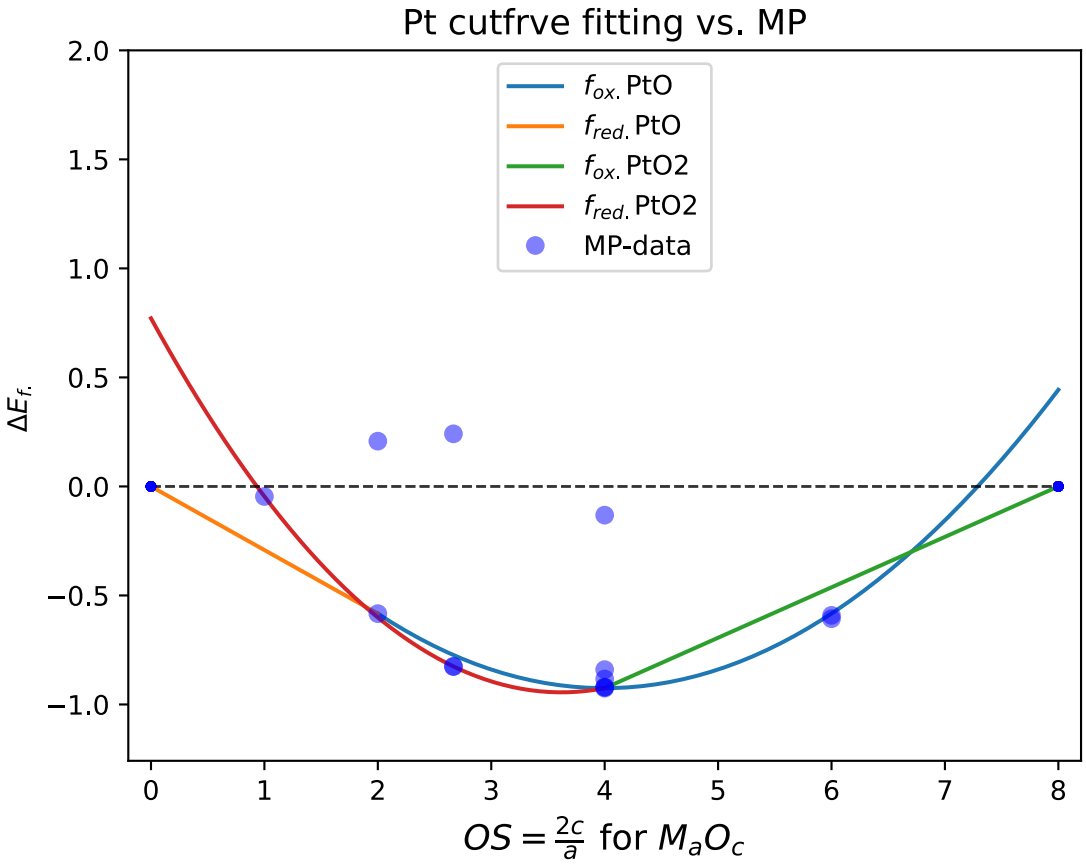

Ni cutfrve fitting vs. MP
$f_{ox.}$ NiO
$f_{red.}$ NiO
$f_{ox.}$ Ni2O3
$f_{red.}$ Ni2O3
$f_{ox.}$ NiO2
$f_{red.}$ NiO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

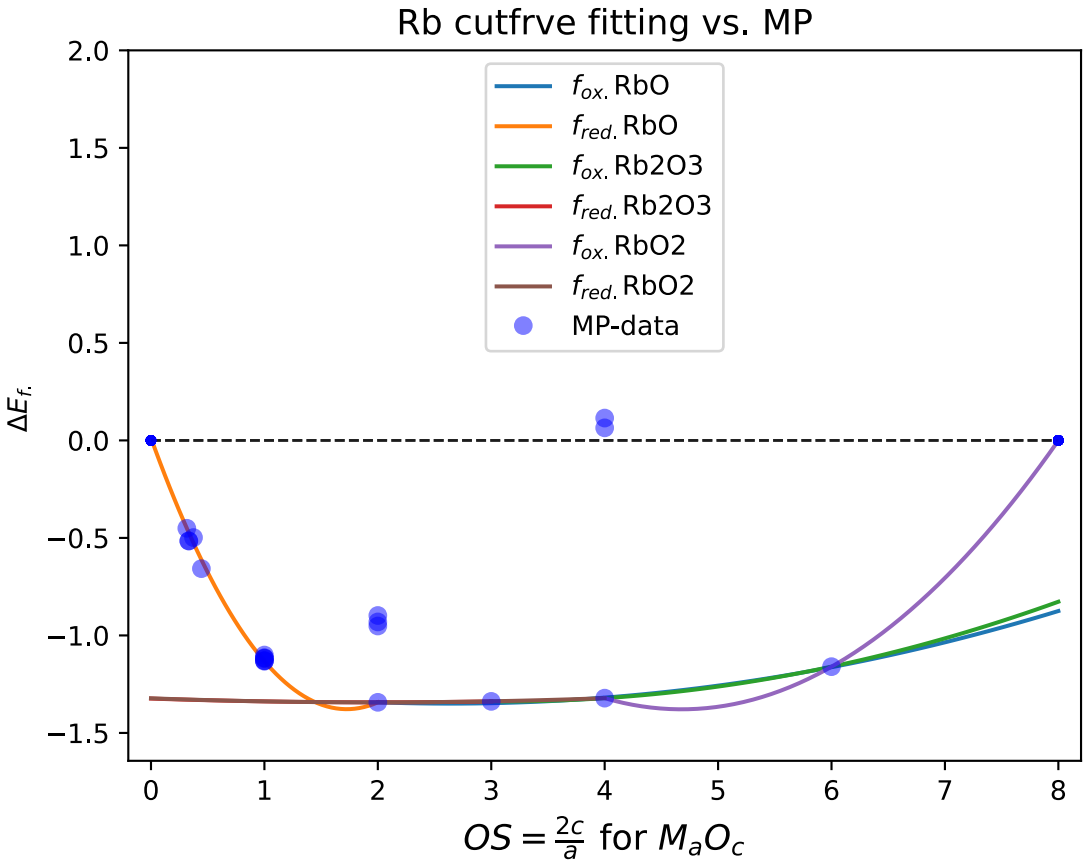

Os cutfrve fitting vs. MP
$f_{ox.}$ OsO2
$f_{red.}$ OsO2
MP-data
$\Delta E_{f.}$
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
0
1
2
3
4
5
6
7
8
$OS = \frac{2c}{a}$ for M_aO_c

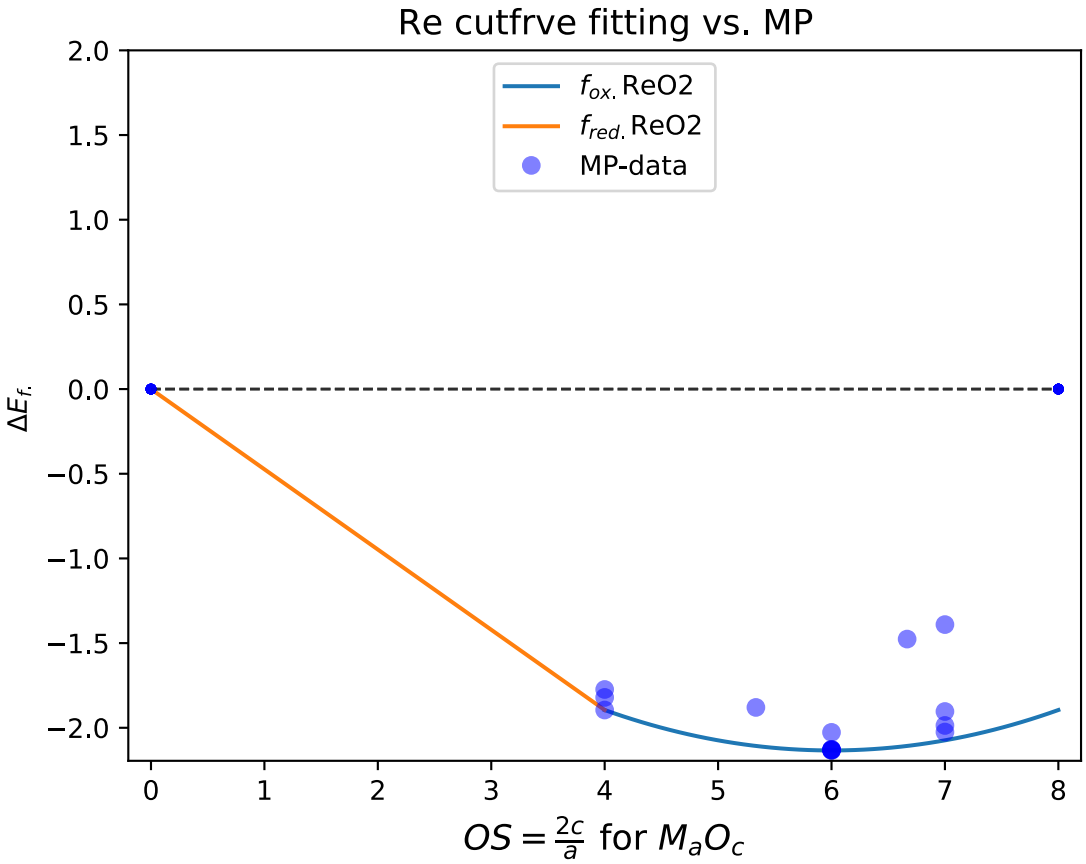

Pb cutfrve fitting vs. MP
$f_{ox.}$ PbO
$f_{red.}$ PbO
$f_{ox.}$ Pb2O3
$f_{red.}$ Pb2O3
$f_{ox.}$ PbO2
$f_{red.}$ PbO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

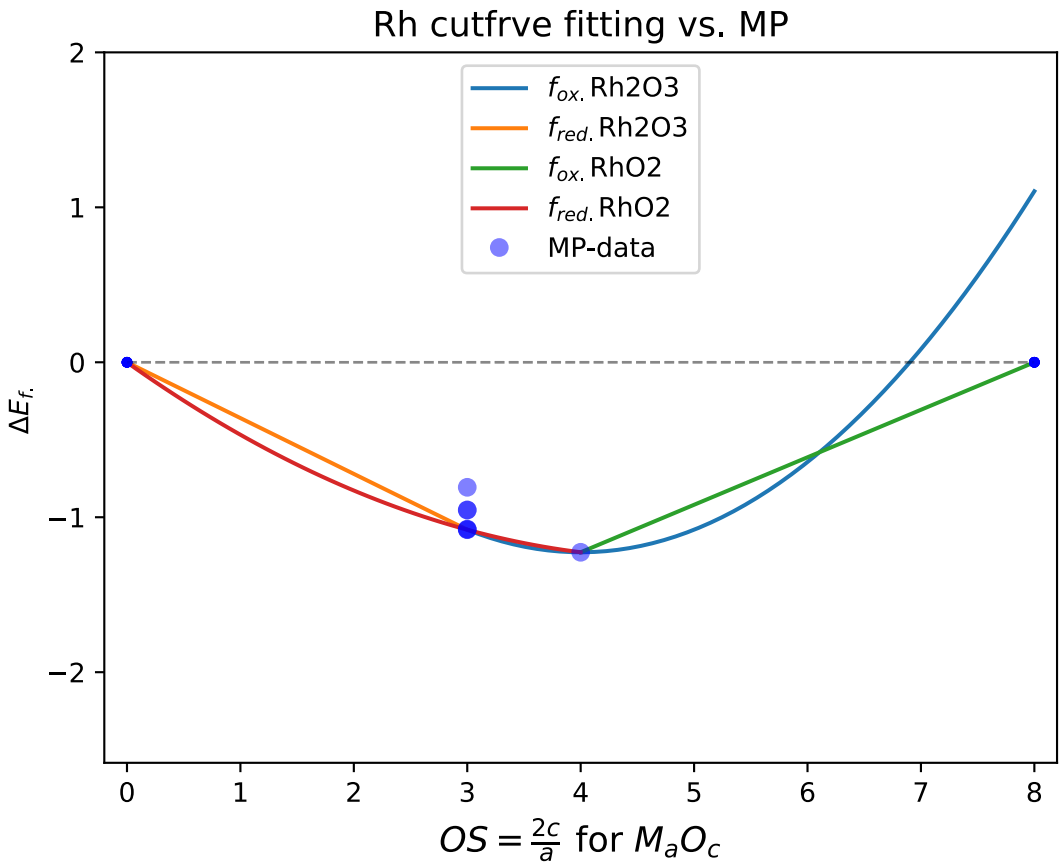

Pd cutfrve fitting vs. MP
$f_{ox.}$ PdO
$f_{red.}$ PdO
$f_{ox.}$ PdO2
$f_{red.}$ PdO2
MP-data
$\Delta E_{f.}$
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
0
1
2
3
4
5
6
7
8
$OS = \frac{2c}{a}$ for M_aO_c

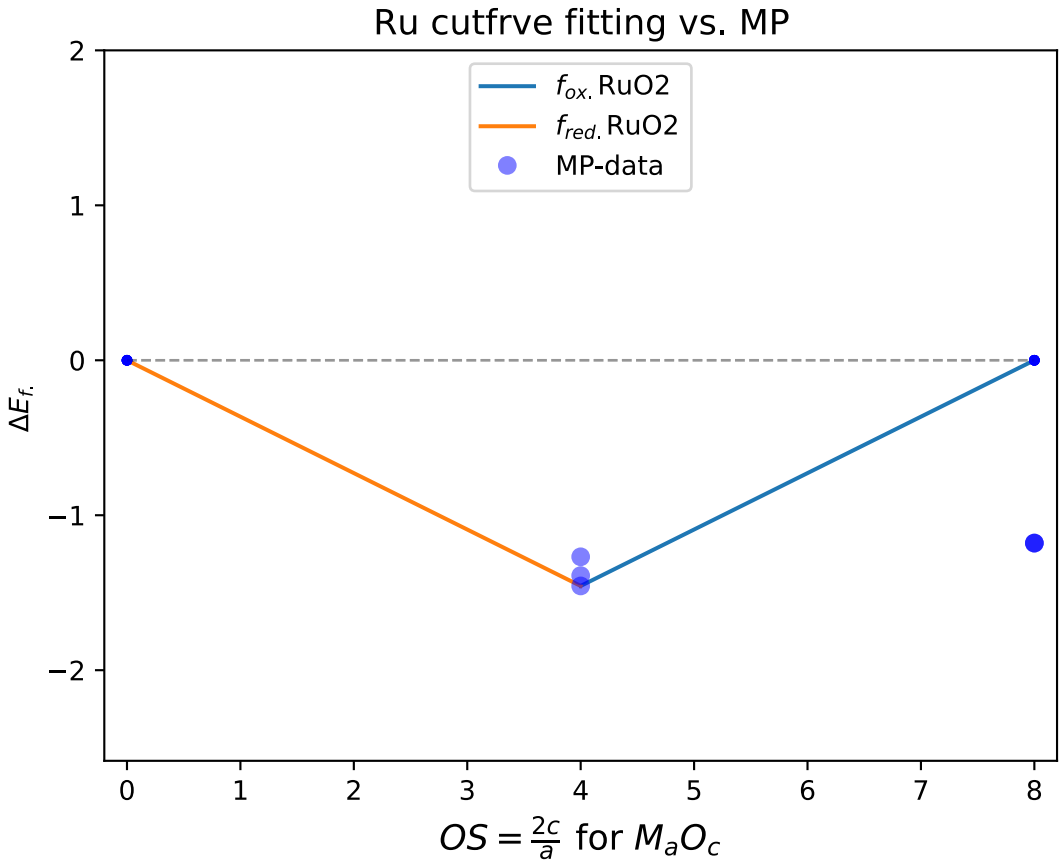

Pr cutfrve fitting vs. MP
$f_{ox.}$ PrO
$f_{red.}$ PrO
$f_{ox.}$ Pr2O3
$f_{red.}$ Pr2O3
$f_{ox.}$ PrO2
$f_{red.}$ PrO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

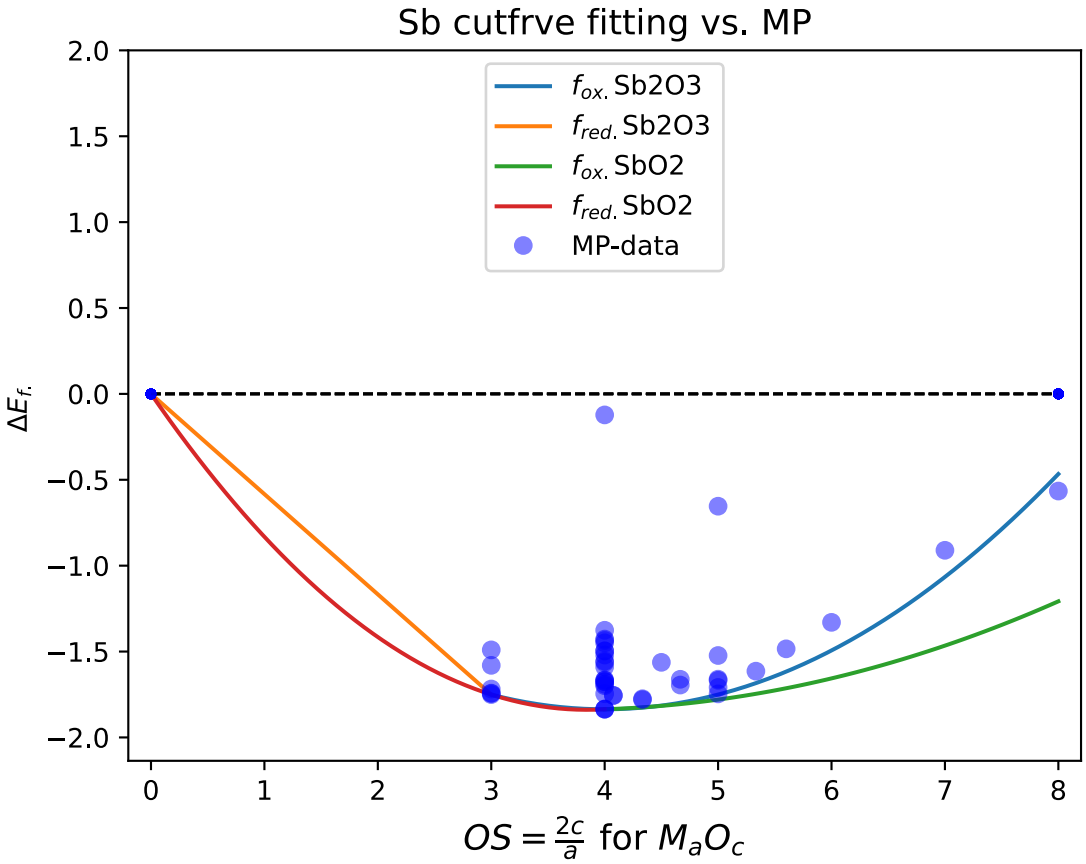

Pt cutfrve fitting vs. MP
$f_{ox.}$ PtO
$f_{red.}$ PtO
$f_{ox.}$ PtO2
$f_{red.}$ PtO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

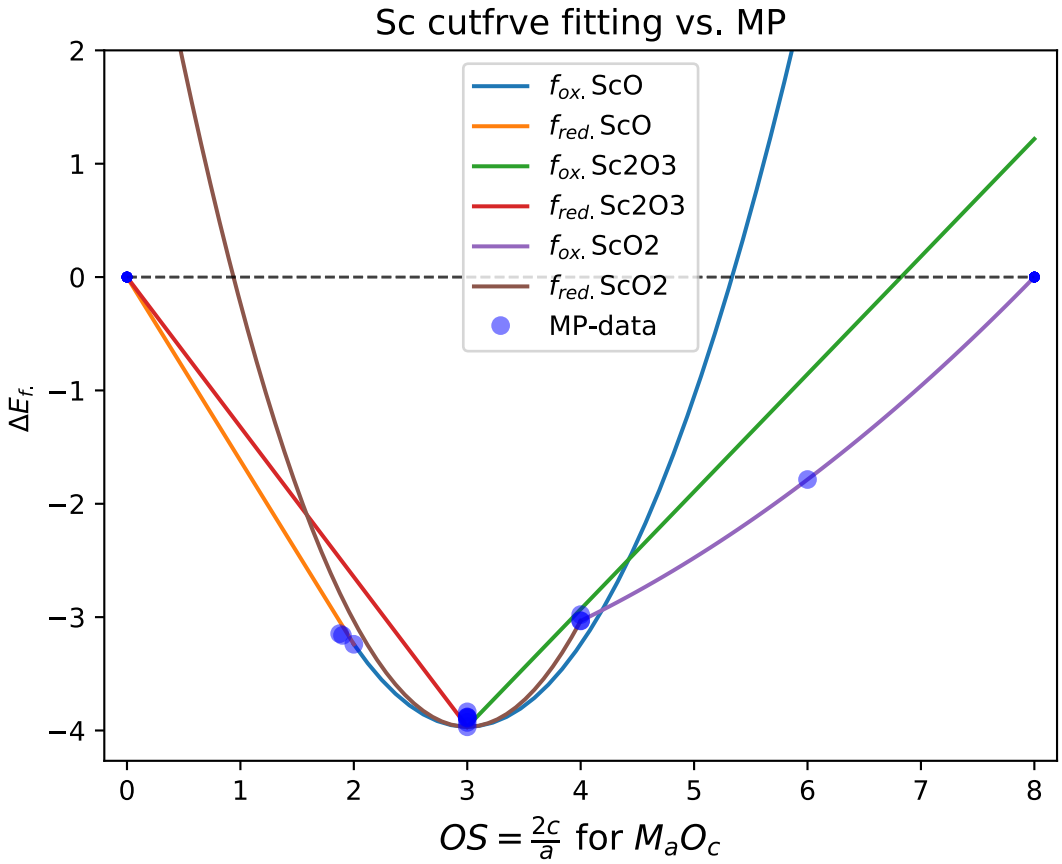

Rb cutfrve fitting vs. MP
$f_{ox.}$ RbO
$f_{red.}$ RbO
$f_{ox.}$ Rb2O3
$f_{red.}$ Rb2O3
$f_{ox.}$ RbO2
$f_{red.}$ RbO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

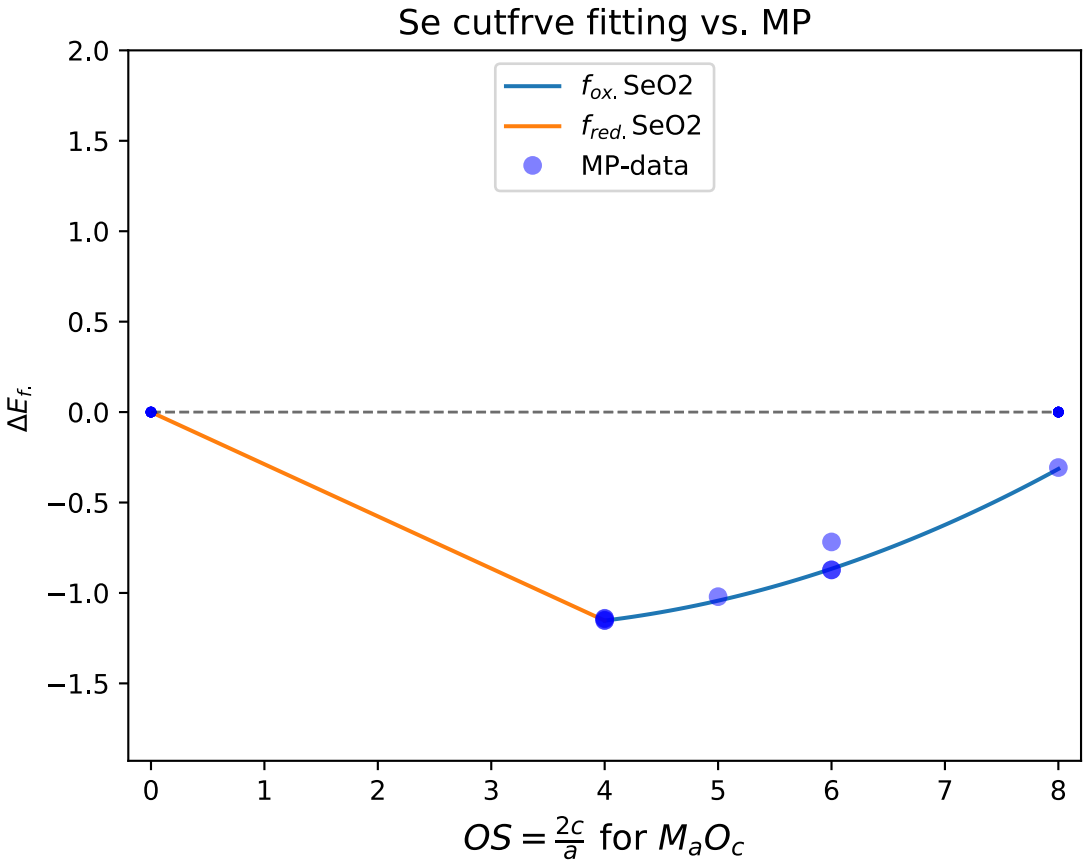

Re cutfrve fitting vs. MP
$f_{ox.}$ ReO2
$f_{red.}$ ReO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

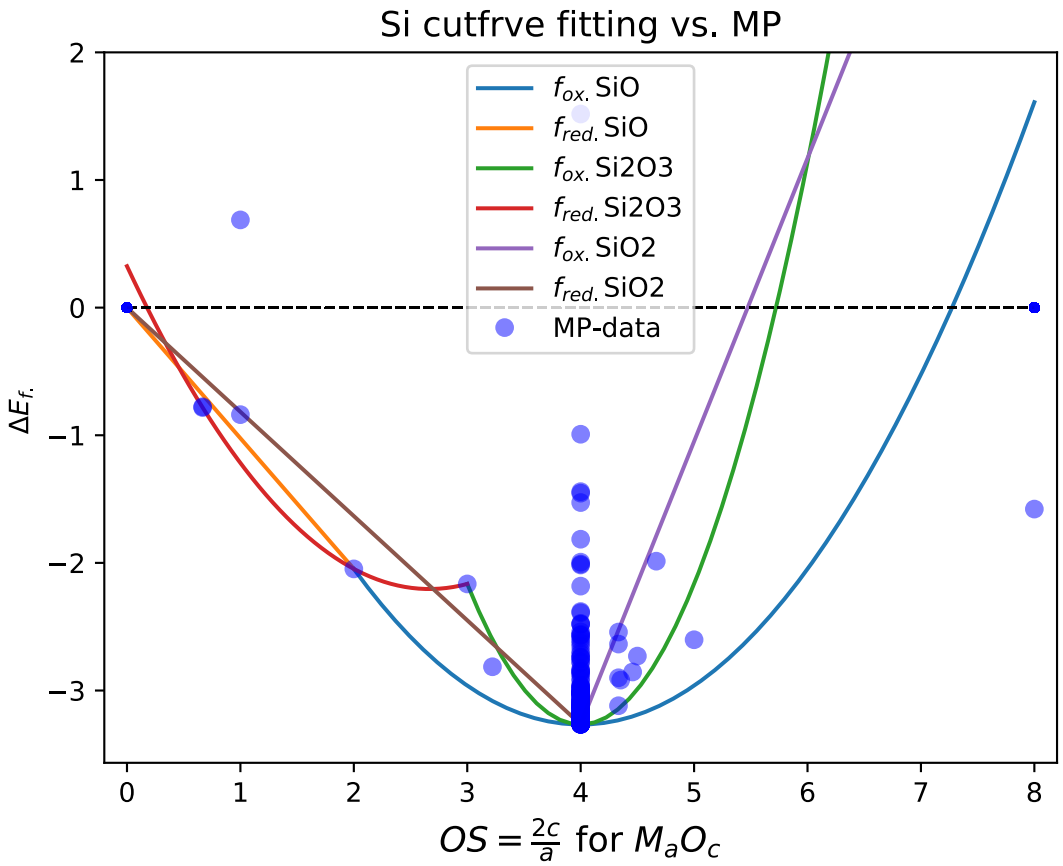

Rh cutfrve fitting vs. MP
$f_{ox.}$ Rh2O3
$f_{red.}$ Rh2O3
$f_{ox.}$ RhO2
$f_{red.}$ RhO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

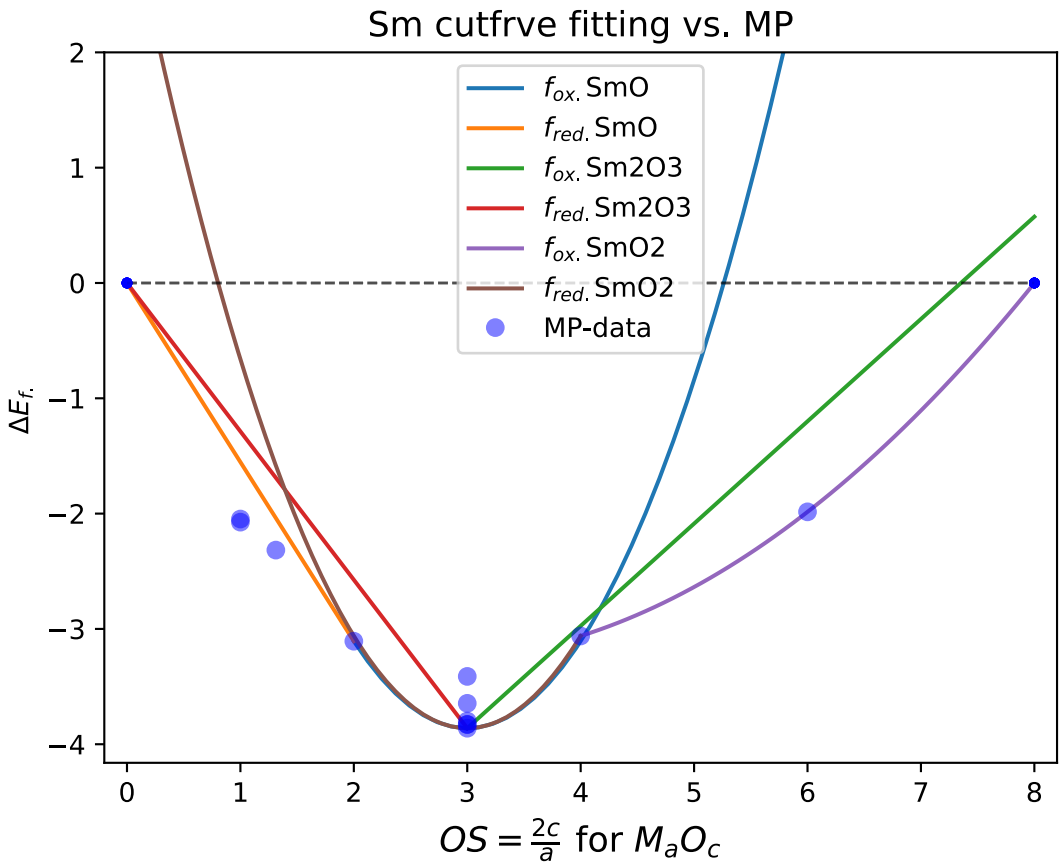

Ru cutfrve fitting vs. MP
$f_{ox.}$ RuO2
$f_{red.}$ RuO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

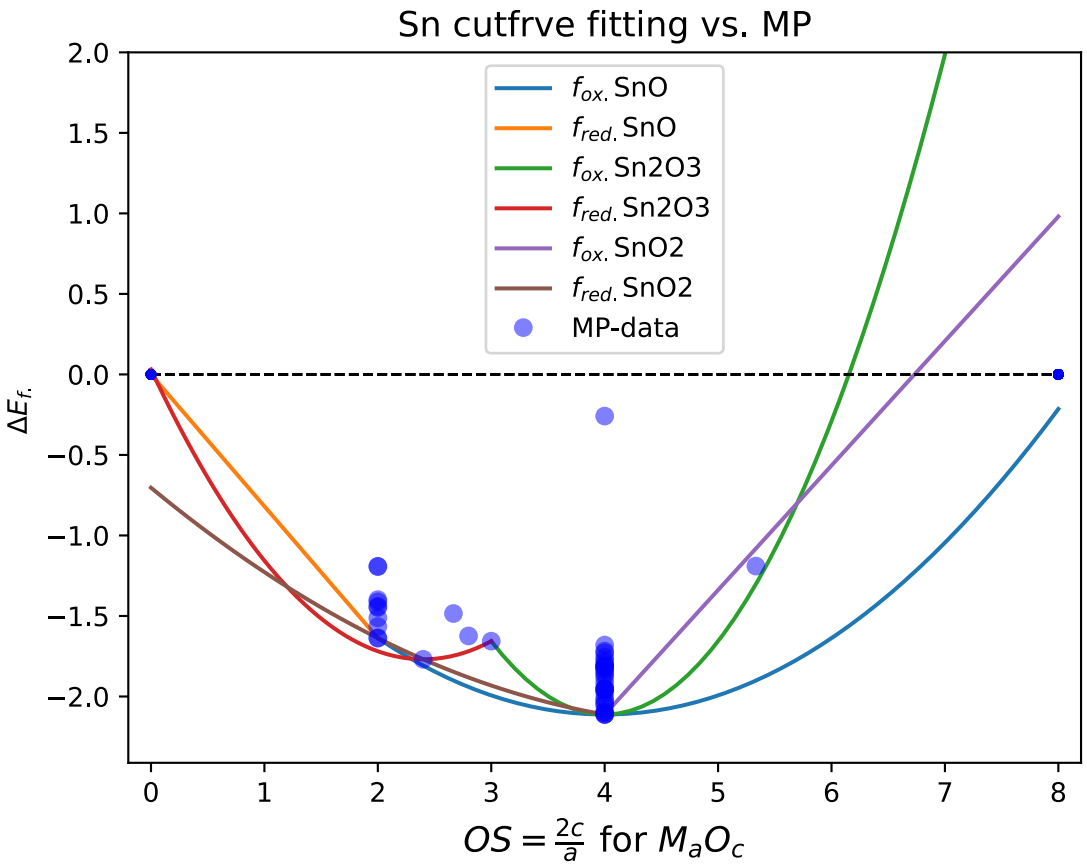

Sb cutfrve fitting vs. MP
$f_{ox.}$ Sb2O3
$f_{red.}$ Sb2O3
$f_{ox.}$ SbO2
$f_{red.}$ SbO2
MP-data
ΔE_f
$OS = \frac{2c}{a}$ for M_aO_c

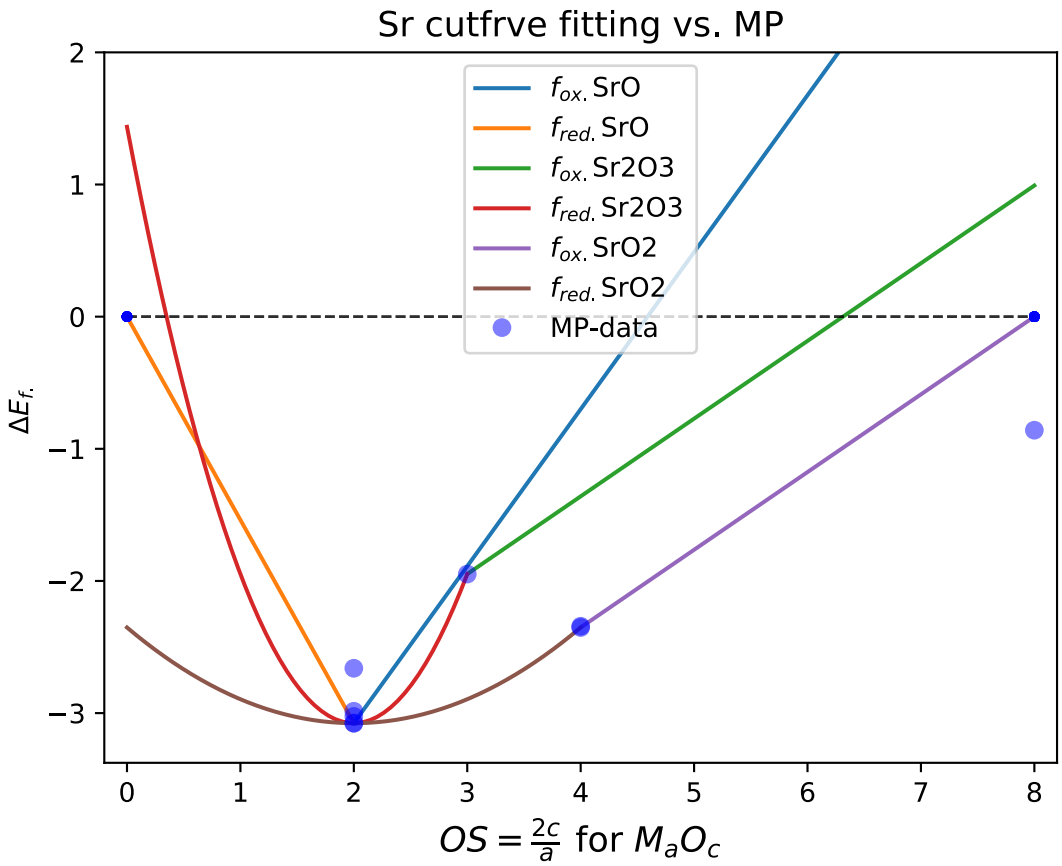

Sc cutfrve fitting vs. MP
$f_{ox.}$ ScO
$f_{red.}$ ScO
$f_{ox.}$ Sc2O3
$f_{red.}$ Sc2O3
$f_{ox.}$ ScO2
$f_{red.}$ ScO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

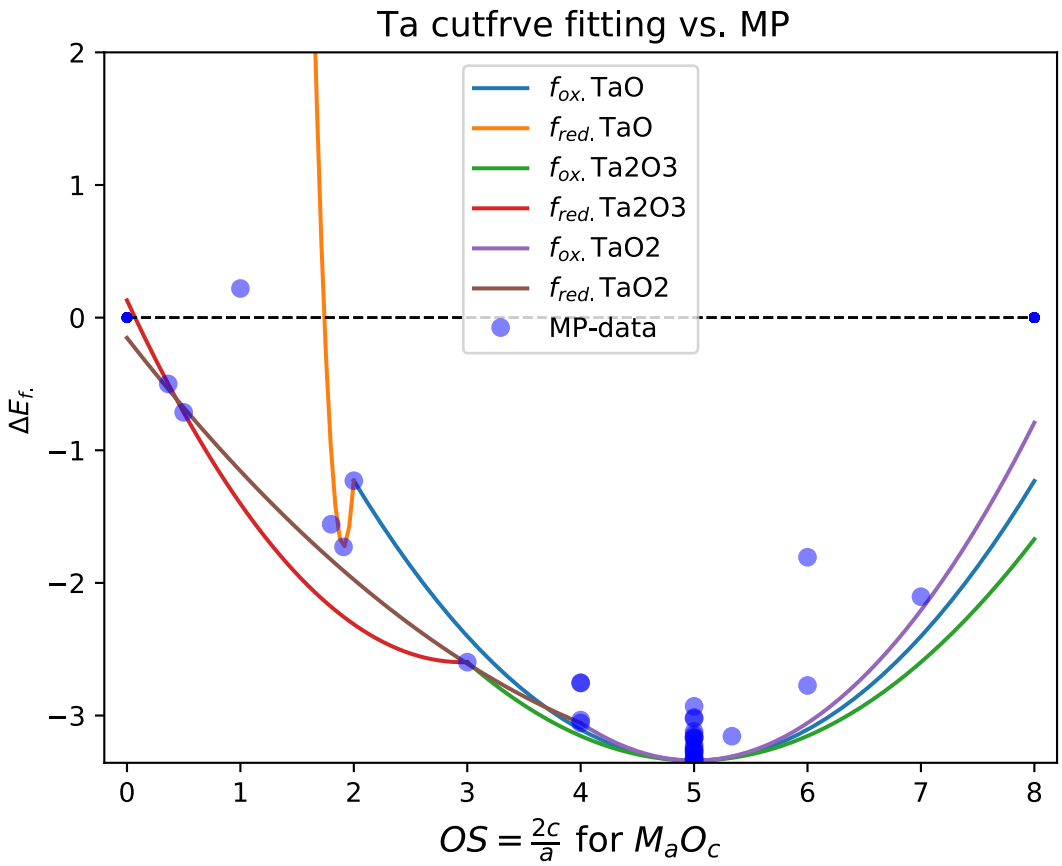

Se cutfrve fitting vs. MP
$f_{ox.}$ SeO2
$f_{red.}$ SeO2
MP-data
ΔE_f.
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
0
1
2
3
4
5
6
7
8
$OS = \frac{2c}{a}$ for M_aO_c

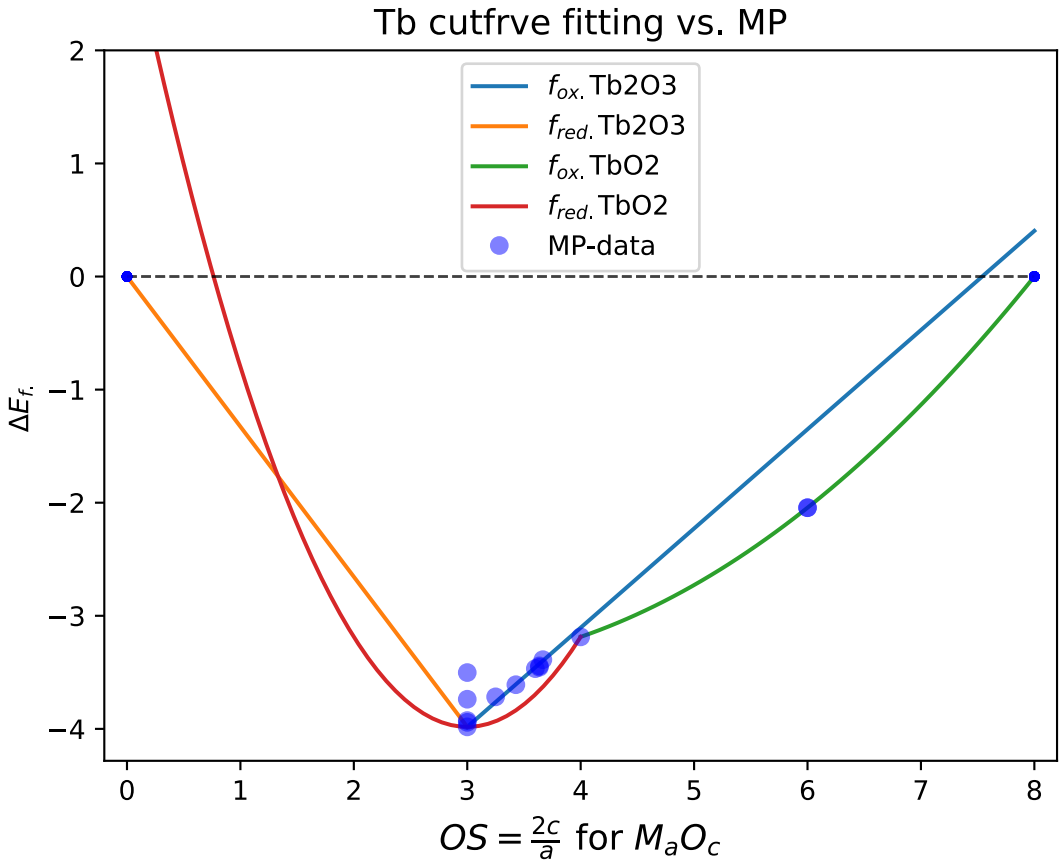

Si cutfrve fitting vs. MP
$f_{ox.}$ SiO
$f_{red.}$ SiO
$f_{ox.}$ Si2O3
$f_{red.}$ Si2O3
$f_{ox.}$ SiO2
$f_{red.}$ SiO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

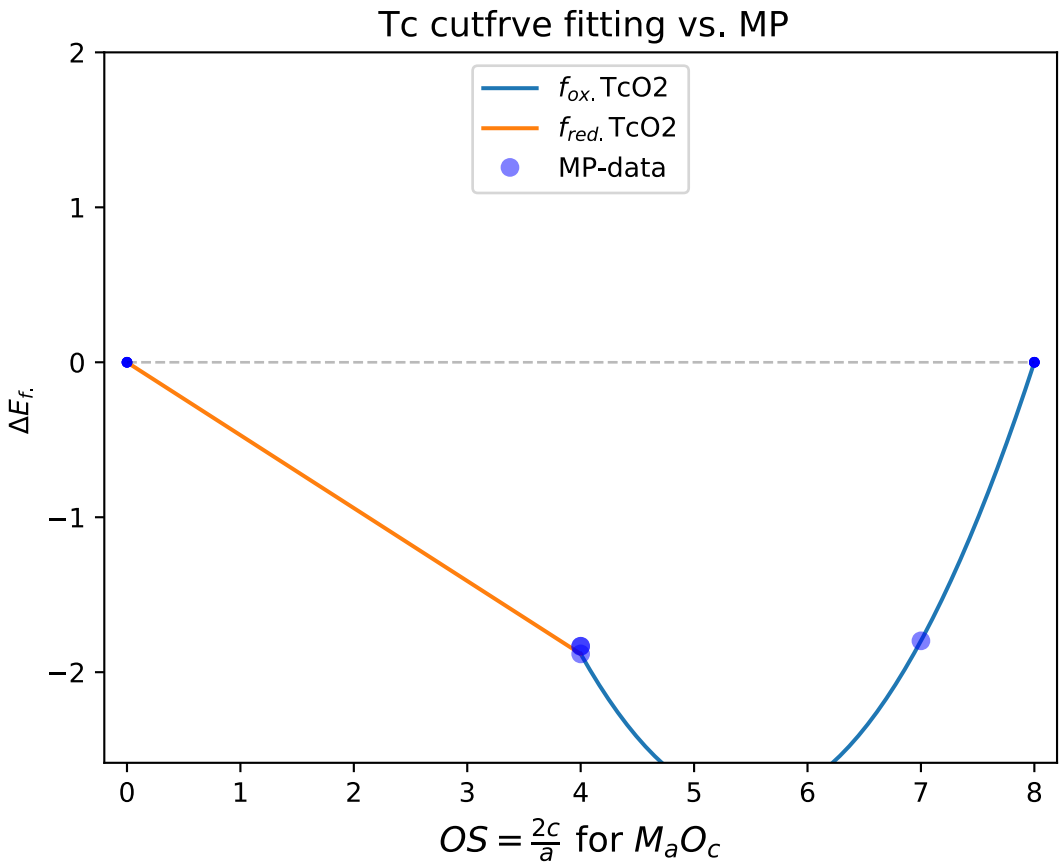

Sm cutfrve fitting vs. MP
$f_{ox.}$ SmO
$f_{red.}$ SmO
$f_{ox.}$ Sm2O3
$f_{red.}$ Sm2O3
$f_{ox.}$ SmO2
$f_{red.}$ SmO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

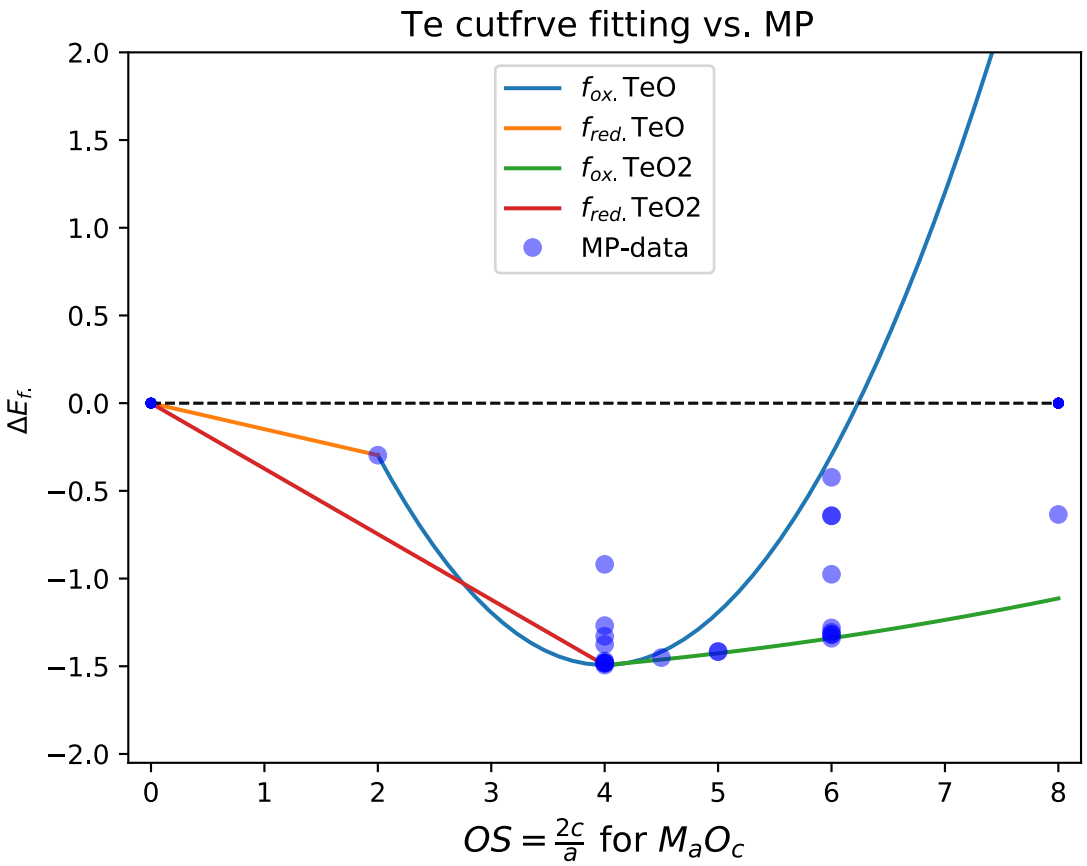

Sn cutfrve fitting vs. MP
$f_{ox.}$ SnO
$f_{red.}$ SnO
$f_{ox.}$ Sn2O3
$f_{red.}$ Sn2O3
$f_{ox.}$ SnO2
$f_{red.}$ SnO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

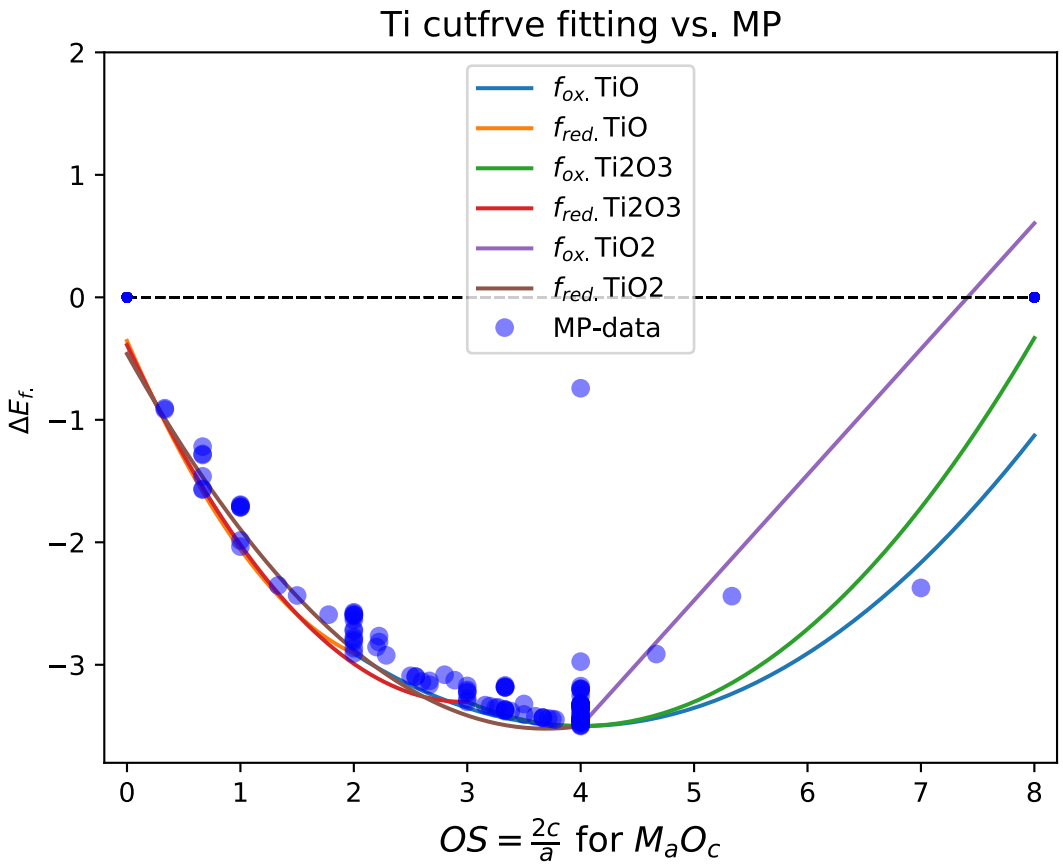

Sr cutfrve fitting vs. MP
$f_{ox.}$ SrO
$f_{red.}$ SrO
$f_{ox.}$ Sr2O3
$f_{red.}$ Sr2O3
$f_{ox.}$ SrO2
$f_{red.}$ SrO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

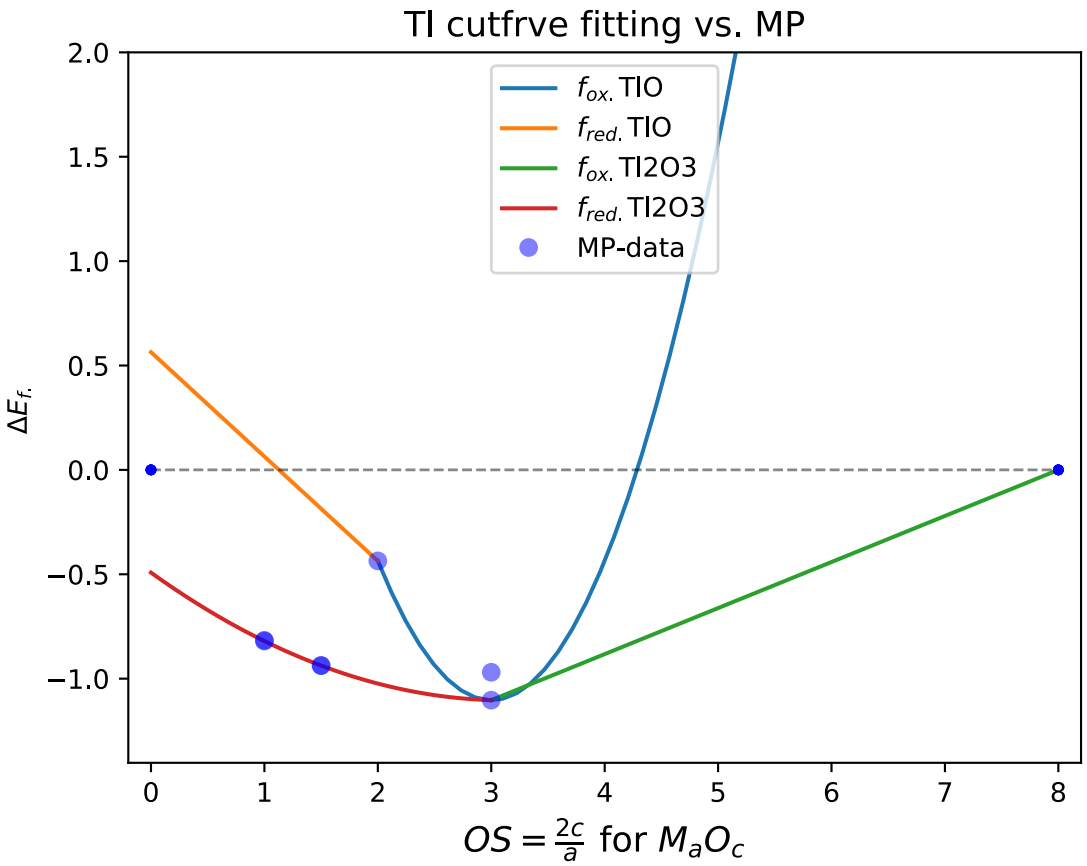

Ta cutfrve fitting vs. MP
$f_{ox.}$ TaO
$f_{red.}$ TaO
$f_{ox.}$ Ta2O3
$f_{red.}$ Ta2O3
$f_{ox.}$ TaO2
$f_{red.}$ TaO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

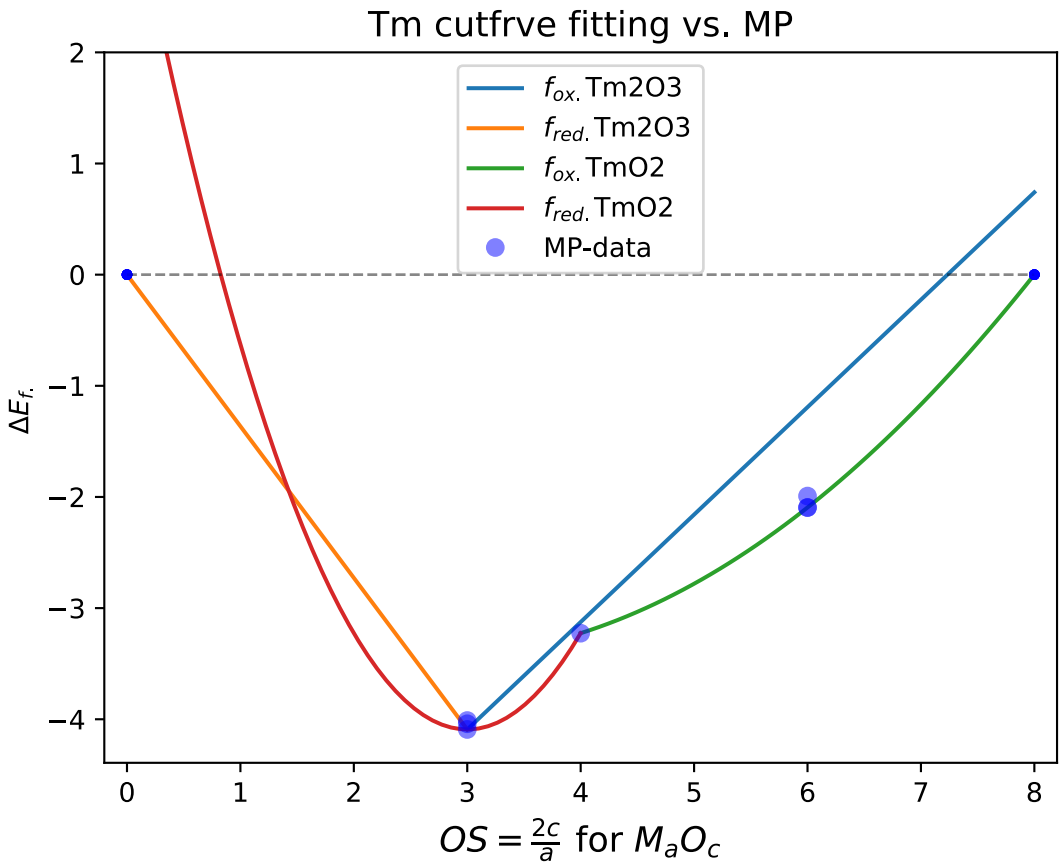

Tb cutfrve fitting vs. MP
$f_{ox.}$ Tb2O3
$f_{red.}$ Tb2O3
$f_{ox.}$ TbO2
$f_{red.}$ TbO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

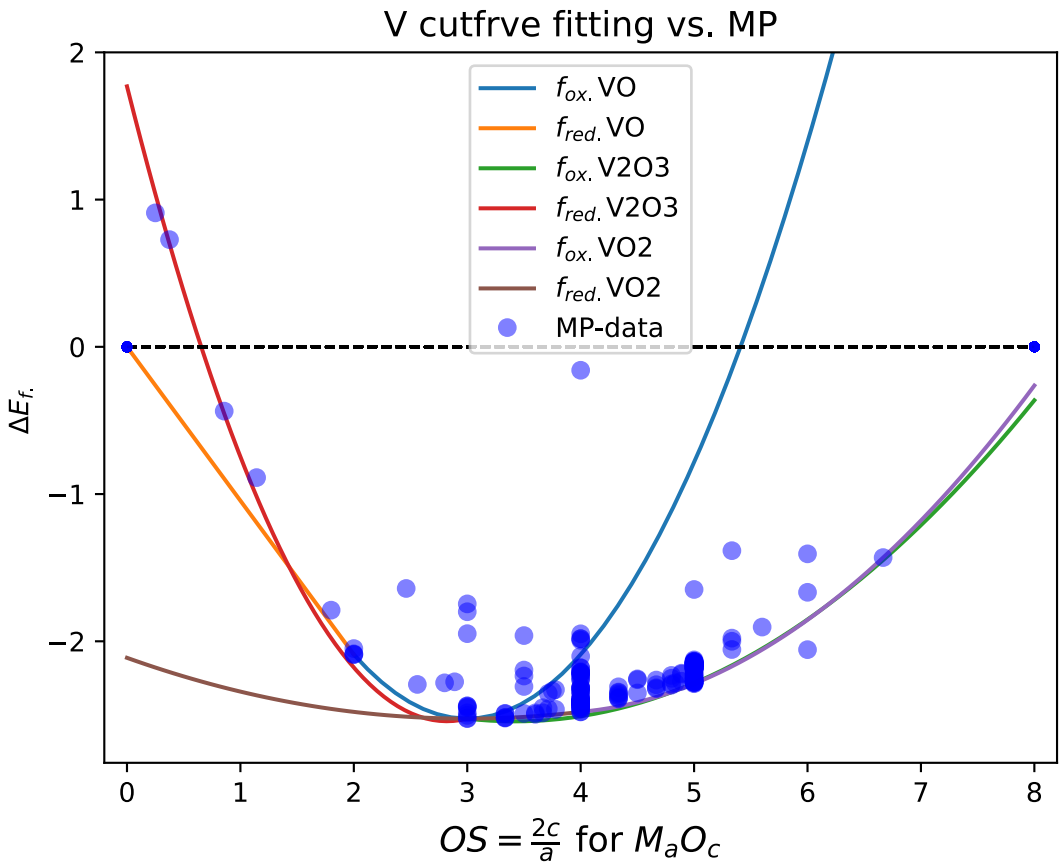

Tc cutfrve fitting vs. MP
$f_{ox.}$TcO2
$f_{red.}$TcO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

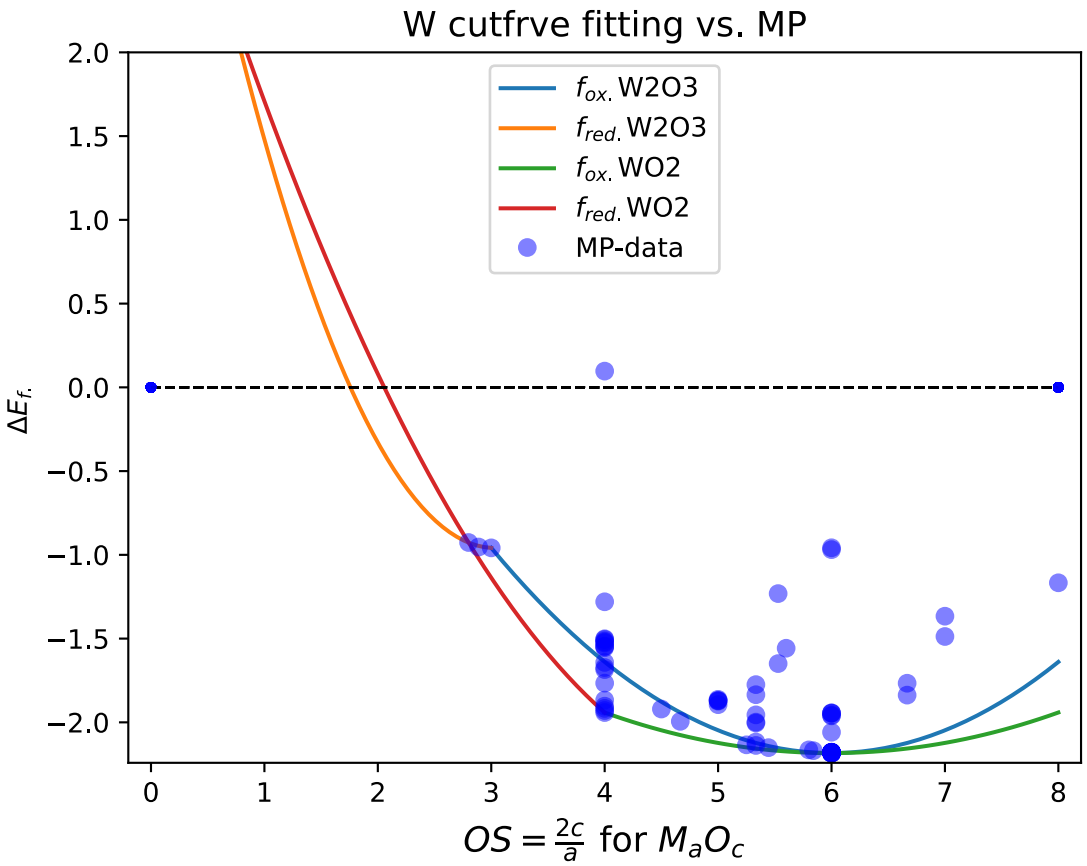

Te cutfrve fitting vs. MP
$f_{ox.}$ TeO
$f_{red.}$ TeO
$f_{ox.}$ TeO2
$f_{red.}$ TeO2
MP-data
ΔE_f
$OS = \frac{2c}{a}$ for M_aO_c

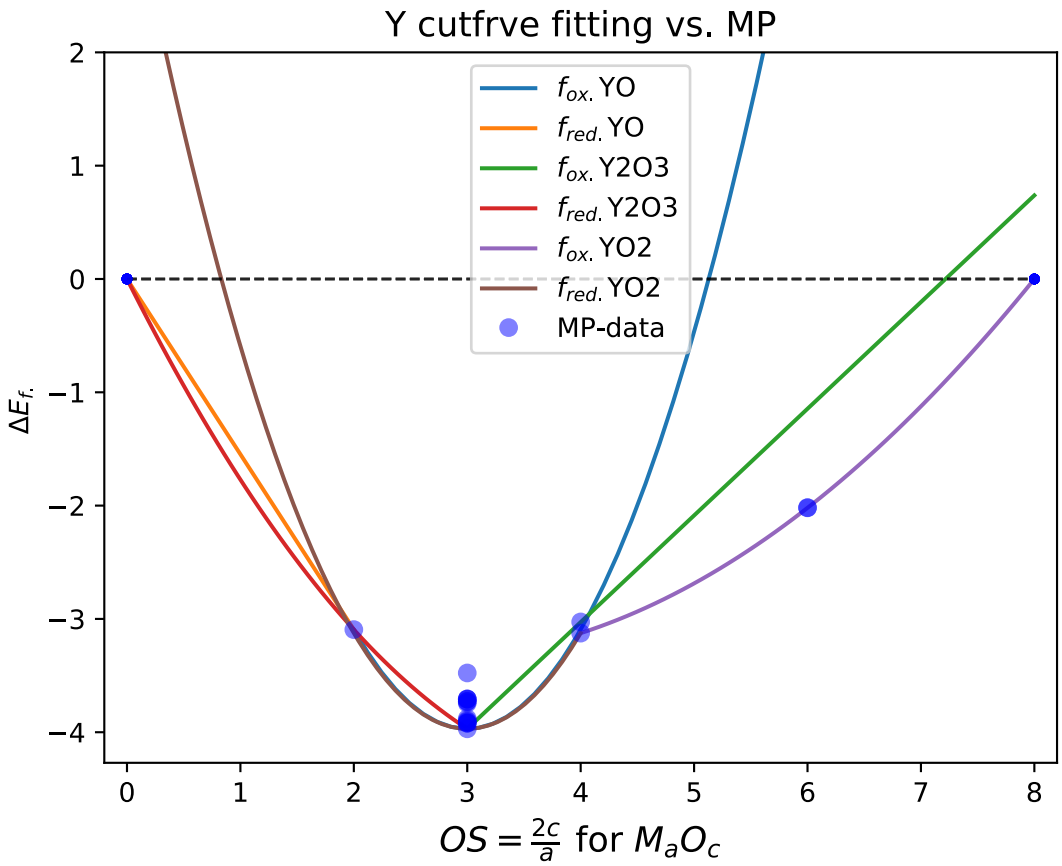

Ti cutfrve fitting vs. MP
$f_{ox.}$ TiO
$f_{red.}$ TiO
$f_{ox.}$ Ti2O3
$f_{red.}$ Ti2O3
$f_{ox.}$ TiO2
$f_{red.}$ TiO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

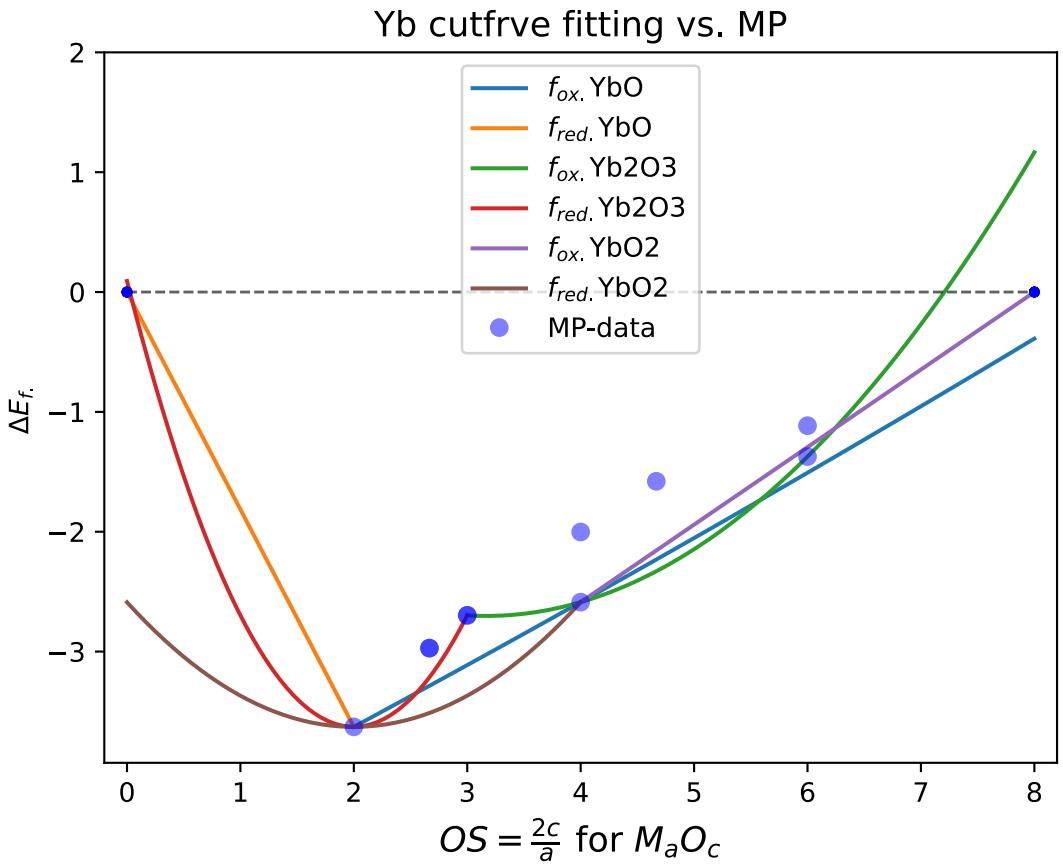

Tl cutfrve fitting vs. MP
$f_{ox.}$ TlO
$f_{red.}$ TlO
$f_{ox.}$ Tl2O3
$f_{red.}$ Tl2O3
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
0
1
2
3
4
5
6
7
8

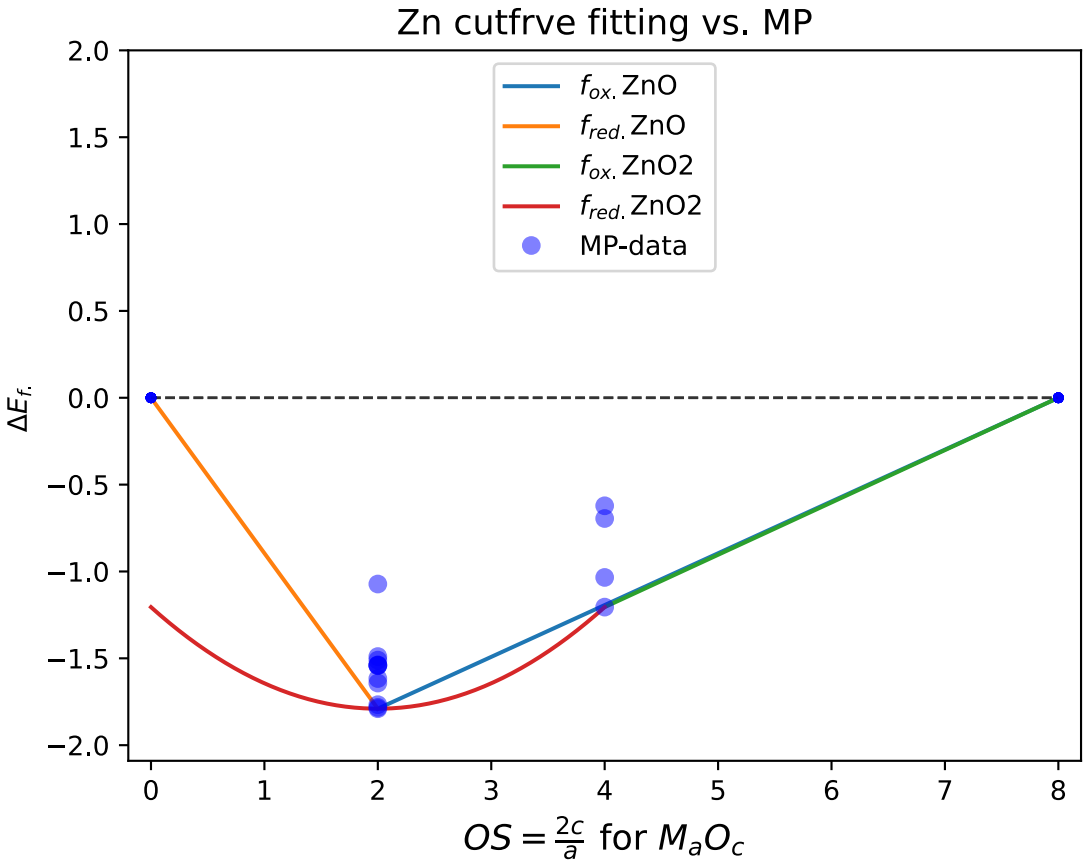

Tm cutfrve fitting vs. MP
$f_{ox.}$ Tm2O3
$f_{red.}$ Tm2O3
$f_{ox.}$ TmO2
$f_{red.}$ TmO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

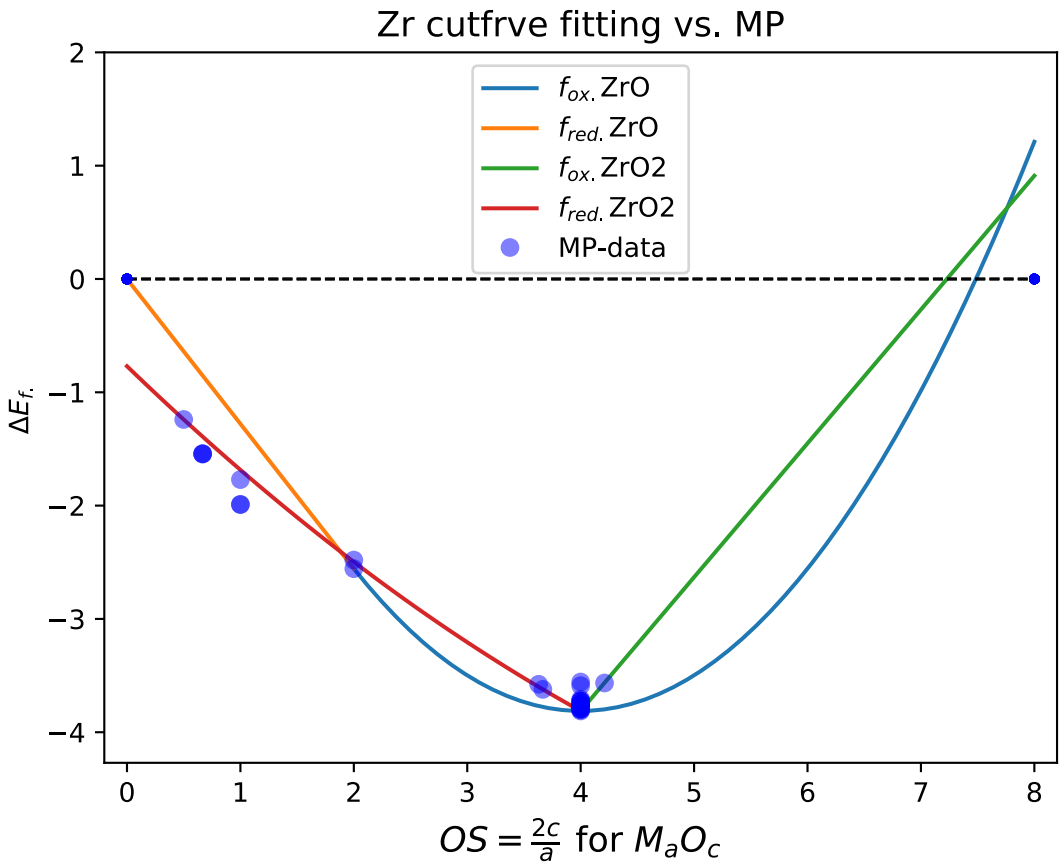

V cutfrve fitting vs. MP
$f_{ox.}$VO
$f_{red.}$VO
$f_{ox.}$V2O3
$f_{red.}$V2O3
$f_{ox.}$VO2
$f_{red.}$VO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c


W cutfrve fitting vs. MP
$f_{ox.}$ W2O3
$f_{red.}$ W2O3
$f_{ox.}$ WO2
$f_{red.}$ WO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c


Y cutfrve fitting vs. MP
$f_{ox.}$ YO
$f_{red.}$ YO
$f_{ox.}$ Y2O3
$f_{red.}$ Y2O3
$f_{ox.}$ YO2
$f_{red.}$ YO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c


Yb cutfrve fitting vs. MP
$f_{ox.}$ YbO
$f_{red.}$ YbO
$f_{ox.}$ Yb2O3
$f_{red.}$ Yb2O3
$f_{ox.}$ YbO2
$f_{red.}$ YbO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c


Zn cutfrve fitting vs. MP
$f_{ox.}$ ZnO
$f_{red.}$ ZnO
$f_{ox.}$ ZnO2
$f_{red.}$ ZnO2
MP-data
ΔE_f
$OS = \frac{2c}{a}$ for M_aO_c


Zr cutfrve fitting vs. MP
$f_{ox.}$ ZrO
$f_{red.}$ ZrO
$f_{ox.}$ ZrO2
$f_{red.}$ ZrO2
MP-data
$\Delta E_{f.}$
$OS = \frac{2c}{a}$ for M_aO_c

3. References

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2. Kirklin, S. *et al.* The Open Quantum Materials Database (OQMD): assessing the accuracy of DFT formation energies. *npj Comput. Mater.* **1**, 15010 (2015).
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