The brief description and flowchart of CE feature construction are described as follows.

1. Define center and environment atom sets.

During the CE feature construction, the atoms in the crystal structure are divided into two atomic sets: the central atoms and the surrounding environment atoms. A and B cation inequivalent sites in the spinel/perovskite structure were chosen as the center atoms, and the environment atoms include the *n*th nearest neighbors from the center atom. In this study, only the first nearest neighbor atoms were considered, which was already proven to be accurate enough to predict the target property in these systems previously.

1. Read the elementary properties of elements.

We selected the 56 elementary properties (Table S1 of the Supporting Information) of elements and pure substances for each constitution element (Figure 1). These elementary properties represent the intrinsic structural and electronic information of the constitution elements of spinel and perovskite oxides, e.g., ionic radius, oxidation state, and electronegativity.

1. Calculate the weights (e.g. reciprocal distances) of environment atoms.

The features of the CE atomic set are composed of the features of the center atom and its environment atoms. In this work the weight of the center atom is a unit, and the weight of the environment atoms is the normalized reciprocal distances (or inversed distances) between the center atom and the environment atoms.

1. Calculate the linear combination of features of environment atoms using weights obtained in step (3).

The given elementary property of the center atom is normally used directly as the feature of that center atom as a scalar (weight is 1). The feature of the environment atoms is a compound property feature assembled using the linear summation of a given elementary property over all environment atoms where the weight of each atom is calculated in step (3).

1. Combine the features of center atoms and environment atoms to construct CE compound feature.

The features of a CE atom set consist of the features of the center atom and its environment atoms in either a scalar or a vector form depending on the manner of assembling these features. For more detailed information, please refer to our previous work [J. Phys. Chem. C, 2020, 124, 52, 28458-28468].

1. Repeat step (1-5) and construct CE features for all center-environment atom sets. Assembly the final CE feature vectors.

Repeat steps (1-5) to generate unique CE features for each structure.



Flow chart of Center-Environment feature construction.