Computational and Experimental Perovskite Redox Materials Design for Solar-Thermochemical Processes

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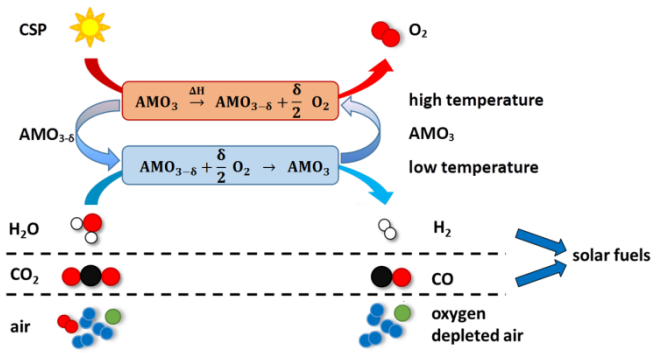

Fig. 1: Thermochemical cycles based on $AMO_{3-\delta}$ perovskites for the production of solar fuels or for air separation. Adapted from [1,2].

Perovskites and their solid solutions are ideal candidate materials for application in two-step thermochemical cycles. By tuning their redox thermodynamics through composition adjustment, ideal perovskite materials can be designed for each type of application, such as fuels production or air separation. Within this presentation, it is shown how these materials can be designed in silico with the help of density functional theory (DFT) and in the framework of The Materials Project. [3] In parallel, some of these perovskite materials are synthesized and their thermodynamic data is fit computationally. By creating a model based on theoretical and experimental data, we screened over 240 perovskite solid solutions and added the results to The Materials Project and as a contribution to MPContribs, the user data portal of The Materials Project. By this means, we created a web interface containing user-interactive graphs, which will be made available freely to the public. The web interface is demonstrated and it is shown how materials can be selected with the help of computational methods based on their redox properties. We are convinced that this data helps accelerate the discovery of new redox materials through bypassing the time-consuming search of materials in the laboratory, which is often based on trial and error.

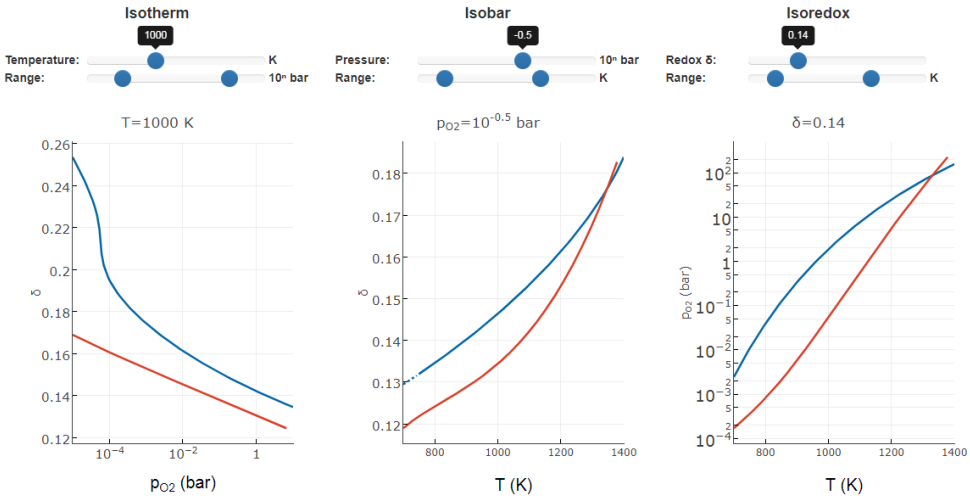

Fig. 2: User-interactive graphs describing the reduction of a (Ca,Sr)(Mn,Fe) perovskite oxide based on its thermodynamics according to theoretical data (red) and experimental data (blue).

References

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