

Objective

We are working to find the optimal formula for the hybrid organic inorganic perovskites (HOIPs) for solar cell energy conversion by using the statistical models to analyze mass data underlying in the published articles.

Hybrid Organic Inorganic Perovskite

The recent years have seen the rapid emergency of a new class of solar cell based on HOIPs. Incorporating perovskites into semiconductor devices such as solar cells has shown good performance. Although the first efficient solid-state perovskite cells were reported only in 2012, a very fast progress was made during five years with power conversion efficiencies reaching a confirmed 20%.

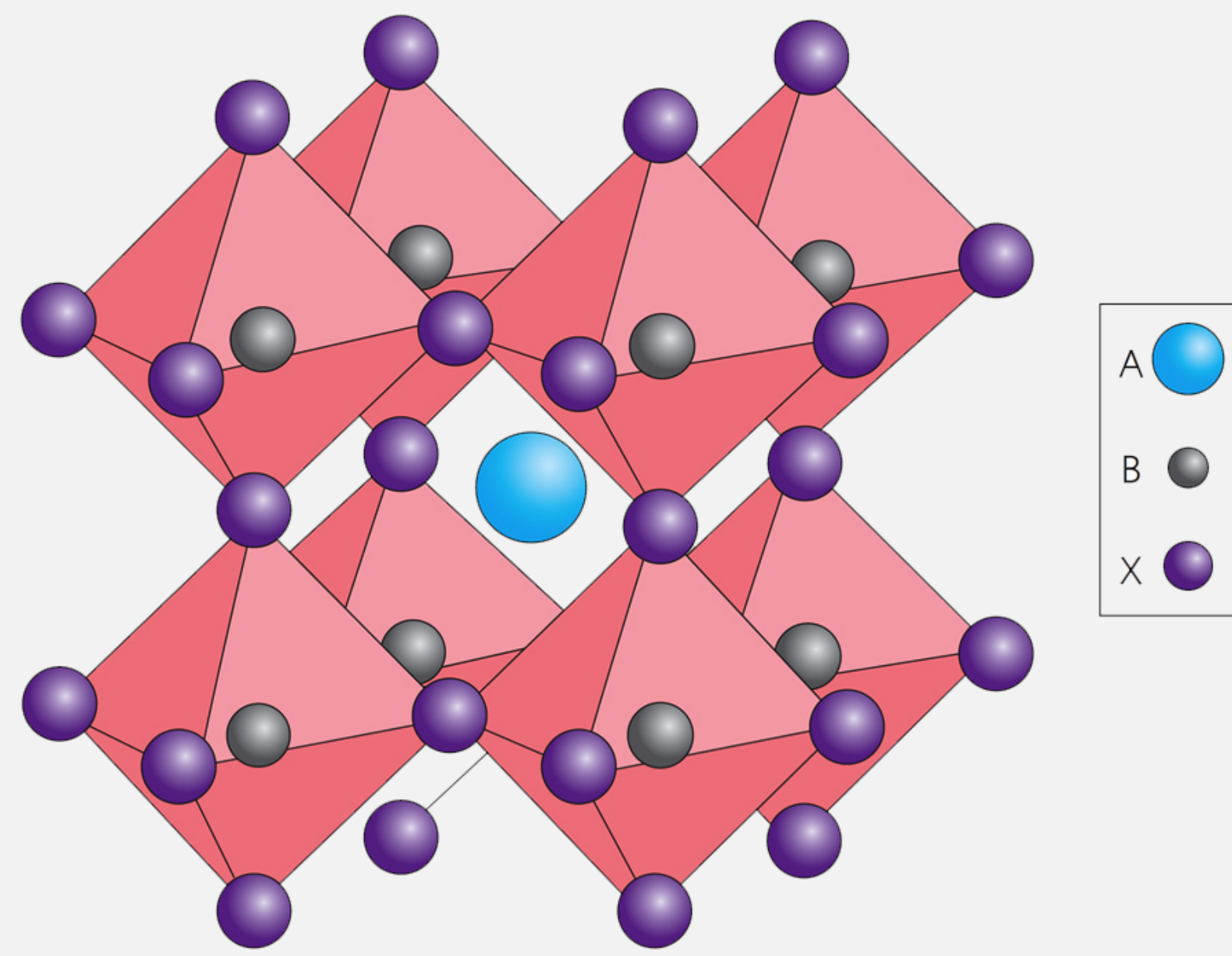


Figure 1: The schematic structure of the ABX₃ HOIP.

Workflow

Though there are a lot of studies in the A/B/X sites mixtures of the HOIPs, they are not stored in a centralized database. We searched related papers from 2015 to 2017, found 250 different formula in about 50 papers.



Figure 2: The workflow of the project.

Optimal Components in the ABX₃ Formula

In the project, the limited amount of data require us to have a efficient data structure to carry on the analysis.

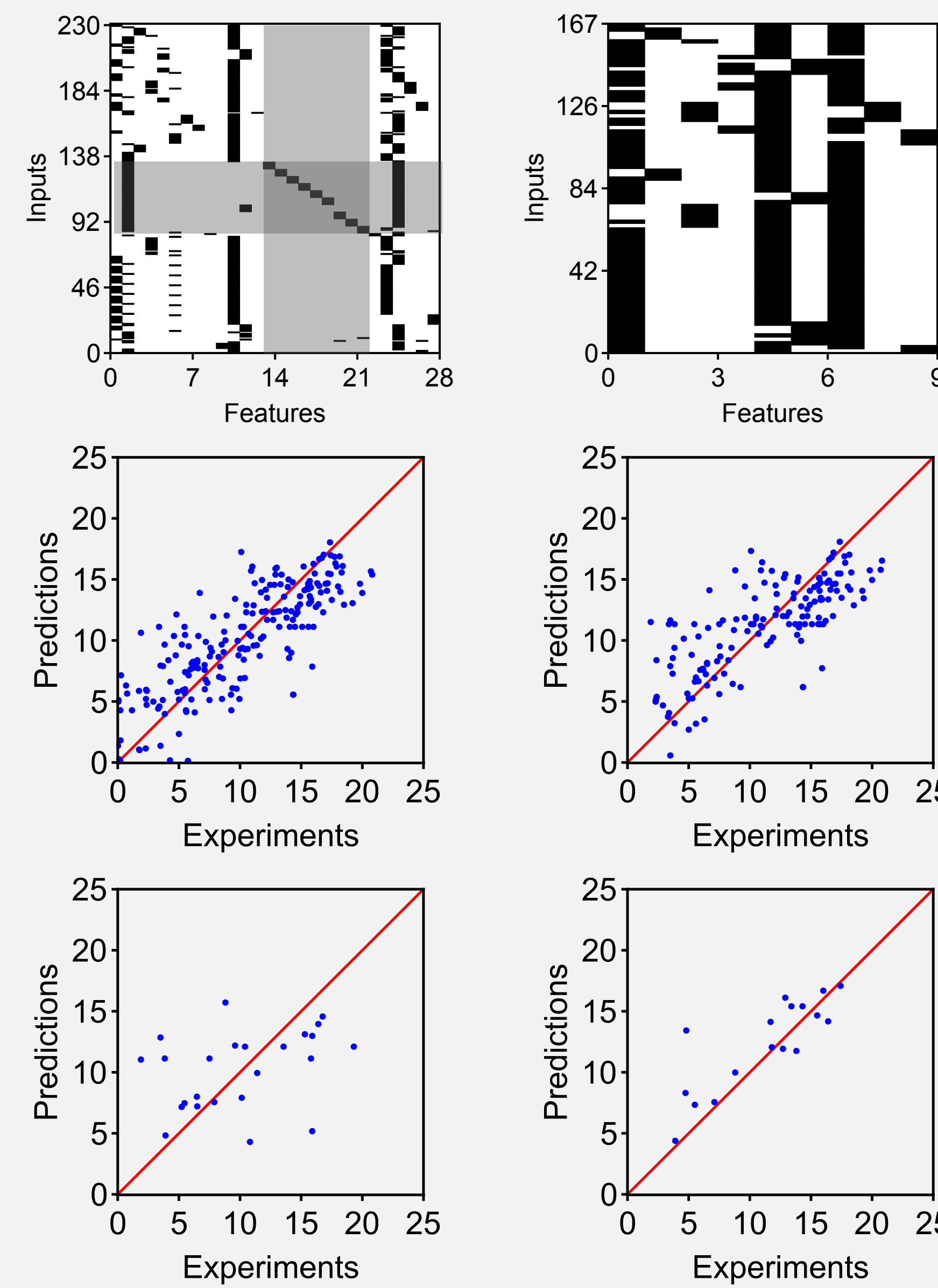


Figure 3: Comparison of Fermi level energies using different methods.

Optimal Components in the ABX₃ Formula

The merit of the linear regression model is to give the inference of each feature to the max PCE.

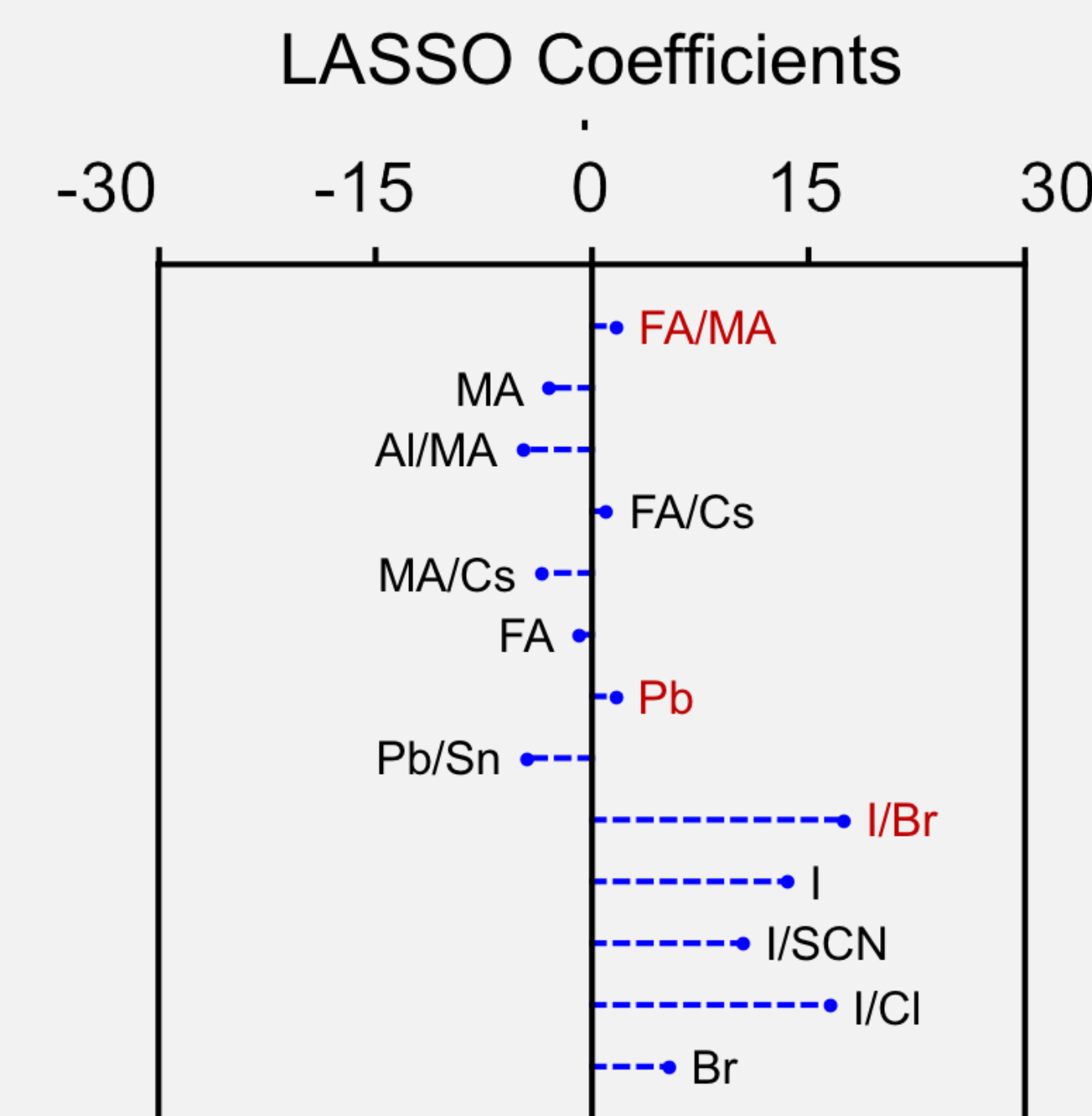


Figure 4: The fitting parameters from the LASSO.

Optimal Ratio of FA/MA and I/Br

Once the optimal components have been determined, we use the back-propagated neural network to fit the PCE response to the component ratio.

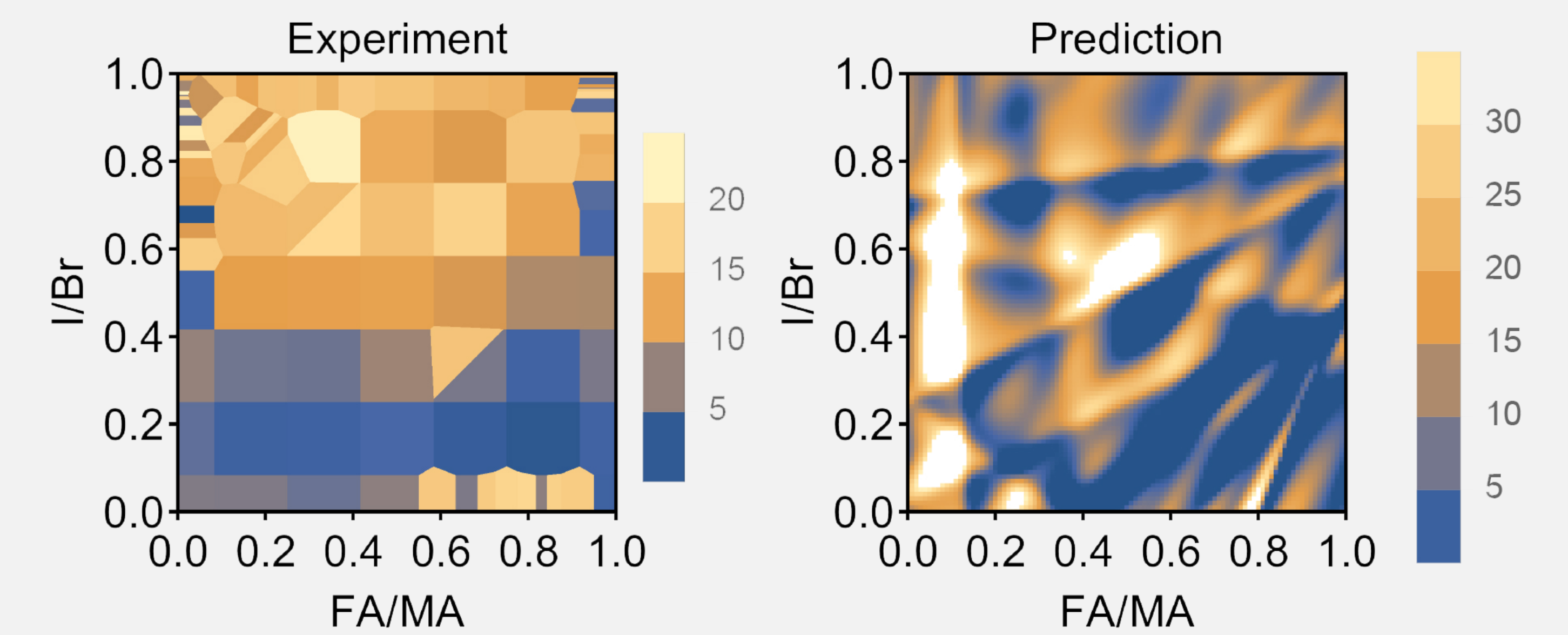


Figure 5: The prediction based on the BP-NN fitting

Conclusion

We have used the data science techniques to identify the optimal combination of elements in the HOIPs for the energy conversion in the solar cells. The lead based HOIP is so far still the best candidates for the solar cell application. A prediction in the wide range of FA/MA, I/Br mixture has been made based on the SVR statistical model.

References

- [1] L. E. Brus, *J. Chem. Phys.* **79**, 1983, 5566.

Acknowledgments

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