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A Computational Approach to Magnesium Corrosion Engineering

Small organic molecules constitute useful materials to modify the service environment of light metals, such as magnesium (Mg). As the lightest engineering metal, Mg is promising for advanced technologies that will tackle climate change through improved battery technologies and advanced transport applications. However, due to its high chemical reactivity, target applications require tailoring of the degradation properties. The vast chemical space of potentially effective compounds can be explored by quantitative structure-property relationship (QSPR) models. We use molecular similarities in a kernel ridge regression model to predict the experimental performance of a large number of chemicals. The model robustness is confirmed by blind validation. Finally, a workflow is presented that facilitates the automated discovery of chemicals with desired dissolution modulating properties.

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