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Selection of Effective Corrosion Inhibitors for Aluminium Alloys based on Data-Driven Techniques

The replacement of highly protective but toxic hexavalent-chromium-based corrosion inhibitors with novel and safer inhibitors for aluminum (Al) alloys is urgently required. Small organic molecules have emerged as safe and potent alternatives showing promising corrosion inhibition for Al alloys [1]. Experimental techniques alone can only screen a tiny fraction of the vast chemical space of available compounds despite tremendous progress in the screening of potential inhibitors by efficient high throughput techniques. Quantitative structure-property relationship models offer the opportunity to preselect a list of promising candidates for experimental testing without in-depth knowledge of the underlying chemical mechanisms. In this work, we used a set of small organic molecules to develop a data driven model to predict their corrosion response for AA2024-T3.

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[1] D.A. Winkler, M. Breedon, P. White, A.E. Hughes, E.D. Sapper, I. Cole, Using high throughput experimental data and in silico models to discover alternatives to toxic chromate corrosion inhibitors, Corros. Sci. 106 (2016) 229-235.

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