A hybrid AI based approach for the optimization of composite coatings development trough electroplating processes

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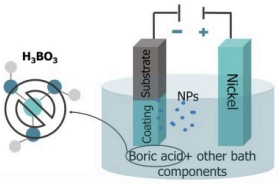
This work presents a methodology relying on Artificial Intelligence (AI) and modelling methods to improve the synthesis of new coating solutions for the surface finishing industry. Such methodology is based on the development of a hybrid dataset composed of experimental data of electroplating processes and also computational models. These models describe the hydrodynamics of the system on the one hand, and the coating deposition on the other. Such dataset is used with two main purposes: first, feeding a Generative Model (GAN) for the design and optimization of the electrolytic bath and second, to feed a Physics Informed System (PINN) that predicts properties of the coating deposition for a set of electrochemical conditions. The present work describes the structure of the dataset and the main approaches followed to construct the GAN and the PINN networks for each case. This methodology represents a remarkable step towards the definition of a safe and sustainable by design (SSbD) framework for the development of composite coatings that can replace hard chromium, known as a toxic component, for applications in manufacturing, machinery and the automotive industry.

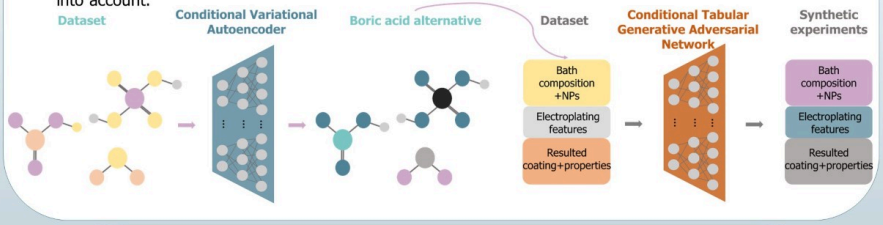
Introduction

- MOZART project proposes nano-composite coatings based on nickel-matrix in replacement of hard chromium-based ones.
- As initial approach Generative Adversarial Networks + Bayesian Optimization were going to be used for helping with the design of the electrolyte bath and coating structures.
- Most of experiments use boric acid as part of the electrolyte bath, which is not sustainable.



Methodology

- Experiments are carried out to find an alternative to boric acid with similar behaviour based on pK_a.
- The initial approach has been changed and a Conditional Variational Autoencoder is being used to find an alternative to boric acid based on its properties.
- After that, a Conditional Tabular GAN will be used for the design of the baths taking the new alternative acid into account.

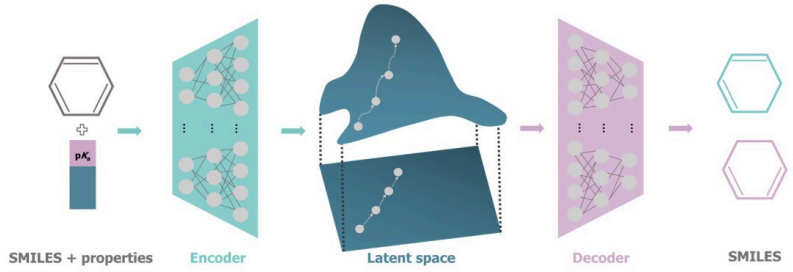


Dataset for CVAE

- ~7000 canonical SMILES of acid molecules.
- pK_a of each molecule.
- To define: other molecule's properties related to pK_a.

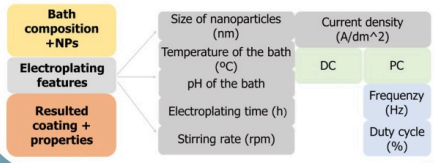
Conditional Variational Autoencoder

- CVAE allows to introduce properties/conditions of the SMILES as input and encode them into latent space.



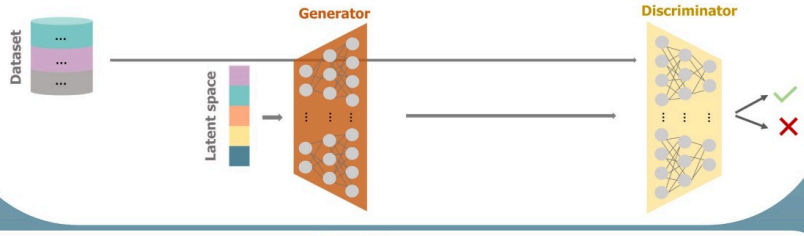
Dataset for CTGAN

- Hybrid dataset of electroplating processes for coating codepositions coming from experiments and simulations:
  - Bath composition + NPs concentration.
  - Electroplating features.
  - Properties and NPs concentration of coating.



Conditional Tabular GAN

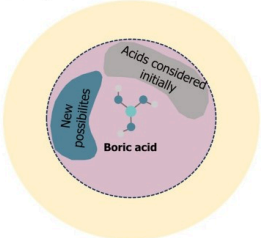
- CTGAN presents some advantages regarding the type of data used for training in comparison to other type of GANs.



Current results

Taking into account a short distance to the boric acid in the latent space:

- Generation of acids not tested experimentally
- Generation of acids that were thought initially as promising candidates



Next steps

- Validation of the results coming from the VAE.
- Definition of a variable that takes into account safe and sustainable design rules to choose the alternative acid.
- Training of CTGAN.
- Development of a Physics Informed Neural Network for prediction of coatings properties given a set of electrochemical conditions.

Aknowledgements

This research has received funding from the European Union's Horizon 2021 research and innovation programme under the project MOZART with Grant Agreement 101058450.

References

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- Zheng, Jonathan W. (2022) IUPAC Digitized pKa Dataset, v1.0. Copyright © 2022 International Union of Pure and Applied Chemistry (IUPAC)