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Electrosorption of a modified electrode in the vicinity of phase transition: A Monte Carlo study

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Graphical abstract



Highlights:

- Monte Carlo simulation was used to study the electrosorption of a electroactive specie on the surface of a modified electrode.
- This model is able to reproduce the main physico-chemical behavior of a on electroactive specie on a modified electrode surface in the presence of a non electroactive species.
- The analysis was based on the study of voltammograms, order parameters, isotherms, configurational entropy per site, in several possible scenarios at different energies and degrees of coverage of non-electroactive species.

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