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Semi-empirical approach to the simulation of molecule-surface reaction dynamics

Migliorini, D.

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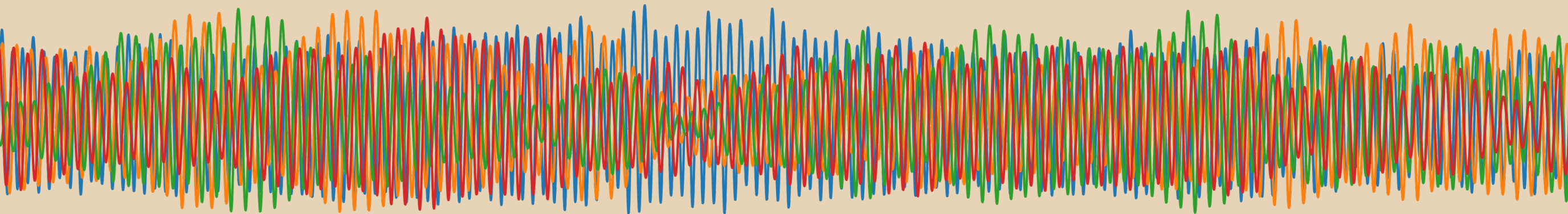
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Davide Migliorini

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