



Swiss Science Concentrates

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Short Abstracts of Interesting Recent Publications of Swiss Origin

Onboard Carbon Capture for Circular Marine Fuels

M. Charalambous, V. Negri, V. Kamm, and G. Guillén-Gosálbez*

ACS Sustainable Chem. Eng. **2025**, *13*, 3919

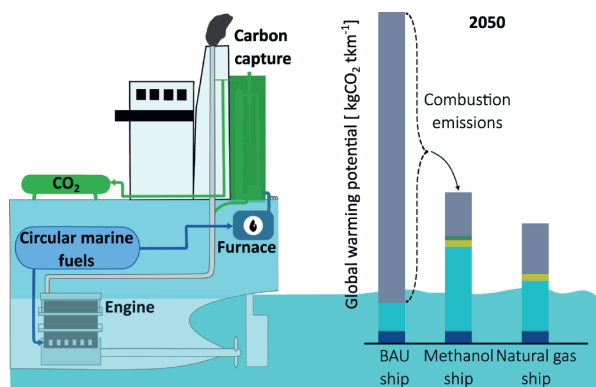
<https://doi.org/10.1021/acssuschemeng.4c08354>

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The transition to low- and zero-carbon fuels is key for reducing emissions in the maritime industry, with methanol and natural gas emerging as leading options. However, both fuels still release greenhouse gas emissions during their use phase. Our study explores how circular economy principles can be applied in shipping to reduce CO₂ emissions. We propose a closed system in which CO₂ is captured onboard ships powered by CO₂ based methanol or natural gas. The captured CO₂ is temporarily stored on the ship and then offloaded at port, where it is combined with electrolytic hydrogen to synthesize the propulsion fuel, thereby closing the carbon loop. We conduct a techno-economic and prospective environmental assessment of these circular marine fuels and compare their performance against the business-as-usual (BAU) scenario of heavy fuel oil-powered ships. Our analysis shows that by 2050, natural gas could cut CO₂ emissions by 65% and methanol by 55%, based on a 91% carbon capture rate. However, the economic cost remains high, at 339 USD per ton of CO₂ abated for methanol and 260 USD for natural gas, with overall operational costs increasing 3–6 times compared to conventional shipping.

Authors' comments:

“Our work highlights circular marine fuels as a promising solution for reducing emissions in shipping, while securing carbon availability in a future where competition for raw materials across sectors will likely be high.”



The Effect of Salt Additives on the Glycine Crystallization Pathway Revealed by Studying One Crystal Nucleation at a Time

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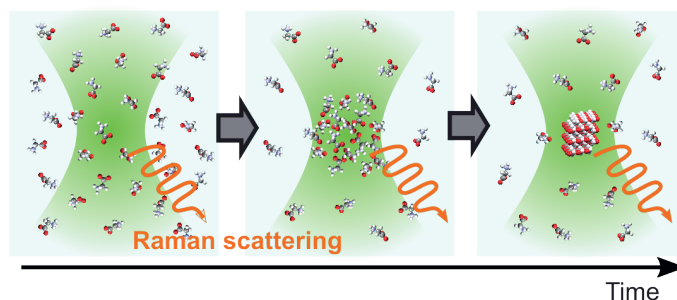
A molecular-level understanding of the early stages of crystallization and the rational control of polymorphism remains a critical challenge in both academic and industrial research. In this study, the effect of sodium chloride (NaCl) on the crystallization pathway of glycine in aqueous solution was investigated using single-crystal nucleation spectroscopy (SCNS), with individual crystallization events observed one at a time. Contrary to the widely accepted mechanism in which γ -glycine nucleates directly in saltwater *via* a classical pathway, it was found that metastable β -glycine forms first through a nonclassical nucleation pathway, both in the presence and absence of NaCl. The β -glycine phase was stabilized by NaCl for several hours and its transformation to α -glycine was inhibited. Over time, γ -glycine was observed to nucleate on the β -glycine surface and grow by consuming the underlying β -glycine crystal. This behavior suggests that stabilization occurs at the polar face of β -glycine and represents a significant advancement in understanding and controlling polymorphism.

Authors' comments:

“This work demonstrates the advantage of SCNS as a new way to study crystallization and the mechanism of polymorph selection. SCNS combined with bulk crystallization study and theoretical approaches will enable the field to achieve the rational design of polymorphism.”

Single crystal nucleation spectroscopy (SCNS)

in situ time-resolved Raman spectroscopy under optical trapping



Determination of Chlorinated Paraffins and Olefins in Plastic Consumer Products of the Swiss Market

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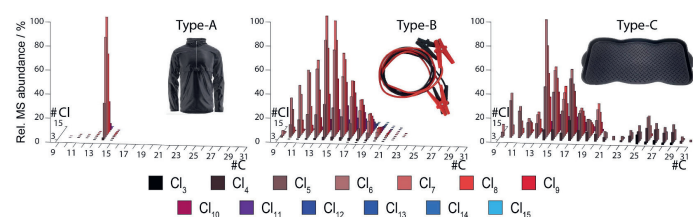
<https://doi.org/10.1016/j.chemosphere.2025.144239>

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Chlorinated paraffins (CPs) are plastic additives under control due to their toxicological and environmental risks. The work from O. Mendo Diaz and colleagues analysed CPs in plastic consumer products from the Swiss market, collected in 2021. A total of 144 samples were pre-screened using GC-ECD, identifying CPs in 32 samples (22%). These were further examined at the homologue level using LC-APCI-Orbitrap-HRMS, with data processed by CP-Hunter. The analysis revealed diverse CP-mixtures, including previously unreported C21- to C31-homologues. Three manufacturing strategies were identified based on the fingerprints: avoiding SCCPs (type-A), using complex CP-mixtures (type-B), and combining CP-mixtures of varying carbon chain lengths and chlorination levels (type-C). A partial SCCP substitution by MCCPs and LCCPs was observed. SCCP levels in 20 samples (14%) exceeded Switzerland's legal limit of 1.5 mg/g. Regular monitoring is recommended to ensure compliance with regulations.

Authors' comments:

“Our recent study highlights how legacy and emerging chemicals of concern such as chlorinated paraffins are often produced, traded, and discarded around us with little oversight. This raises concerns about invisible, uncontrolled contamination.”



Neural Network Potential with Multiresolution Approach Enables Accurate Prediction of Reaction Free Energies in Solution

Felix Pultar, Moritz Thürlemann, Igor Gordiy, Eva Doloszeski, and Sereina Riniker*

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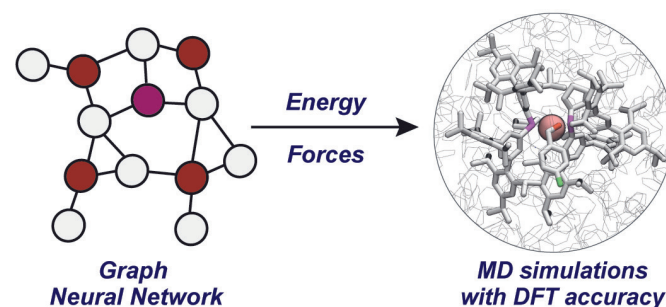
<https://doi.org/10.1021/jacs.4c17015>

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The work from Riniker *et al.* presents a novel neural network potential (NNP) called Anisotropic Message Passing (AMP) combined with an electrostatic embedding scheme, designed to enhance quantum-mechanical/molecular-mechanical (QM/MM) simulations. The AMP model reduces computational costs by replacing expensive QM Hamiltonians with accurate NNPs, enabling efficient molecular dynamics (MD) simulations for large systems. AMP leverages equivariant neural networks to encode symmetries and directional interactions, achieving chemical accuracy (4.184 kJ mol⁻¹) in predictions compared to density functional theory (DFT). The model's performance is demonstrated through applications such as determining ligation states of nickel phosphine complexes and predicting dissociation free energies of charged pyridine-quinoline dimers. Results show excellent agreement with experimental data, outperforming traditional QM/MM simulations with semiempirical methods and static DFT calculations. The AMP architecture scales well, handling systems with over 350 solute and 40,000 solvent atoms, and is computationally efficient, making it suitable for future applications in (bio-)chemical simulations.

Authors' comments:

“Many relevant problems in chemistry are impacted by solvent and conformational effects. The accuracy and computational efficiency of the AMP/MM approach enables us to treat them explicitly in computational studies.”



alanine dipeptide, nickel complexes, pyridine dimers

>100'000 times faster than DFT calculations