Special Issue

Self-Optimizing Purification: Digital Twins, Chemometrics, and Control in Membranes, Adsorption, and Chromatography

Message from the Guest Editors

Submissions are invited on digital shadows and digital twins synchronized with laboratory, pilot, demonstration, or plant data. Relevant topics also include chemometric and soft-sensor methods for hidden-state inference, first-principles and hybrid models for online monitoring, model updating under drift, uncertainty-aware optimization, supervisory decision support, model predictive control, and validated closed-loop strategies. Application settings may include water treatment, gas purification, carbon capture, and down-stream bioprocess purification, provided that the central contribution concerns the operation of the purification step itself. The aim of this Special Issue is to assemble a focused body of work that clarifies which sensing, modeling, and control strategies are sufficiently mature for trustworthy self-optimizing purification and where the principal barriers to deployment still remain.

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About the Journal

Message from the Editor-in-Chief

Purification is international, peer-reviewed, open access journal offering a platform for theories, emerging technologies, and practical applications focused on purification across chemistry, biology, chemical and environmental engineering, materials science, pharmaceutical technology, food engineering, and related disciplines. Due to ongoing advances in purification science, novel materials and regulatory frameworks have emerged, as well as new technical and societal challenges. By bringing together researchers in sustainable manufacturing, environmental remediation, biotechnological innovation, and other emerging fields, Purification fosters open, high-quality research exchange and accelerates the development of related sustainable solutions.

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