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2D materials assisted membrane crystallization: A new combined theoretical and experimental approach

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In the field of nanotechnologies, nano-composite membranes [1-2] enriched with two-dimensional (2D) materials are attracting interest in various areas of the scientific research, due to their peculiar and exceptional electronic properties. Actually 2D materials are becoming promising in membrane technology dedicated to water treatment as well. Specifically, 2D materials confined in defined volumetric spaces can assist mass transfer through membranes under specific conditions. New mechanisms are envisaged to control water sequestration from ion solutions causing quicker ion aggregation processes during Membrane Crystallization (MCr). The latter is part of the membrane technology enabling recovery of valuable salts from seawater and brine. In the recent past [1,3-4], atomistic simulations have provided a detailed picture of the formation of the critical nucleus of salts in supersaturated solution. Herein, for the first time we explore the potential of 2D materials in MCr technology from experimental and computational points of view. A combined molecular approach has been employed to predict and validate the effects of 2D materials on salts nucleation and growth rate when NaCl solution comes in contact with membrane surfaces. Experimental tests and simulations have been performed using different concentrations of exfoliated 2D flakes, designing three different models: pristine PVDF, PVDF with Graphene at 5% wt and PVDF with Graphene at 10% wt. As a first outcome, MD simulation demonstrate how the chemical composition of the membrane surface, can affect the crystallization of salts, while experimental test yield clear the role of the filler in nucleation grow rate, crystal size and shape, but also in the energy of the system [5]. In the overall, the nanomaterials influence kinetics of crystal formation, reducing the nucleation times.

Recent Publications

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2. Perrotta ML, Saielli G, Casella G, Macedonio F, Giorno L, Drioli E, Gugliuzza A (2017) An ultrathin suspended hydrophobic porous membrane for high-efficiency water desalination, Appl. Mat. Today, 9, 1-9.
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Biography

Maria Luisa Perrotta, Ph.D Student at Institute of Membrane Technology of National Research Council (CNR-ITM), has her experience in membrane technology. At first she focused the attention on preparation, characterization and testing of nano-composite membranes in membrane processes (MD and MCr). In the last year she extended her interest in Molecular Dynamics Simulation in order to study at molecular level the behavior of membranes prepared, and also to compare with experimental test. At the moment she is studying Membrane Crystallization process (MCr). The basic aim of this work is to evalue the possible contribute of 2d nanomaterial, used like filler in these polymeric membranes, in crystals growth .

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