[P2.088]

Polyoxometalates in polymer membranes for a more efficient fouling treatment: A nanoscale modeling

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Fouling is undoubtedly one of the major drawbacks limiting membrane-based technology in wastewater treatments. Polyoxometalates display several properties as antibacterial and capability to evolve oxygen from H_2O_2 dismutation[1]. $[PMo_{12}O_{40}]^{3-}$ and $(Ru_4(SiW_{10})_2$ polyoxometalates were suggested as fillers in membrane coatings prepared by a PBM method[2]. The exchange of $[PMo_{12}O_{40}]^{3-}$and $Ru_4(SiW_{10})_2$ with ions on surfaces functionalized with ammonium surfactants (QAS) is herein presented. Since an efficient exchange of bromide with a $[PMo12O40]^{3-}$ definitely increases the antifouling efficiency of the membranes, this exchange was simulated at nanoscale level using a Quantum and Molecular Mechanics [3] approach. The modelling predicted that this exchange takes place in a limited extent[3] due to the low QAS surface concentration and the counter ion used to neutralize the surfactant charge, crucial points to guarantee the electrostatic interaction of the $[PMo12O40]^{3-}$on the surface. *Ad hoc* measures were performed using homemade membranes and analytical measurements, performed to assess the extent of the exchange, are in good agreement with the modeling predictions.

The $Ru_4\,(SiW_{10}\,)_2$ release from PBM coatings results in the reduction of antifouling which is due to the oxygen evolution from the coatings. The second nanoscale modelling is aimed to predict the release of $Ru_4(SiW_{10})_2$, bounded *via* noncovalent bonds to QAS, in solutions containing ions. The QM/MM simulations were performed considering dilute solution of NaCl. The modeling shows that although the QAS-$Ru_4(SiW_{10}\,)_2$ adduct is very stable, the permeation of the target ions in the membrane coating can destabilize this complex.

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Acknowledgment The work performed has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement **No 689427** for the project **VicInAqua**.

Keywords: Nanoscale modeling, Polyoxometalate fillers, Membrane coatings, PBM