Thermodynamic approach for the electrochemical properties of perfluorinated sulfonic membrane : Applicability of simulation technique

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We introduce the molecular thermodynamic approach that combines with atomistic simulation technique. In general, many parameters of binary systems are determined by fitting thermodynamic and electrochemical model with experimental data. In this study, we obtained all parameters using molecular simulation. To take the specific interaction into account, we assume that it only occurs between a solvent molecule and a specific group. We constructed the amorphous cell and performed the dynamics module to achieve the diffusion coefficient and binary interaction parameters in consequence of molecular simulation. Our theoretical approach is worthy of notes that shows the combining of thermodynamic model and computational simulation becomes a realistic possibility to express the real system.