



Impact of dispersion forces on the release dynamics of dissolved gases

Johannes Fiedler (1,2), Clas Persson (2), Stefan Buhmann (1,3)

(1) Institute of Physics, University of Freiburg, Germany (johannes.fiedler@physik.uni-freiburg.de), (2) Centre for materials science and nanotechnology, University of Oslo, Norway, (3) Freiburg institute of advanced studies, University of Freiburg, Germany

The dynamical behaviour of dissolved gas molecules, such as methane and carbon dioxide, at the ocean-atmosphere interface is of great interest to current research. An understanding of fluxes through such interfaces significantly affects environmental research and the hot topic of carbon storage. Typically, the balance of dissolved gases are described via Henry's law that includes the internal partial pressure of the constituents within an infinite bath of solvent. However, close to an interface additional forces have to be taken into account resulting in a deviation from this law. For neutral particles, the additional forces arising due to the presence of an interface are dispersion forces [1] coupling to the polarisability of the particles. In the presence of the environmental medium, in this case water, these interactions have to be modified by the corresponding excess polarisabilities [2]. We introduce a method to describe these effects and present our results for methane and carbon dioxide. We will show a reduction of the release dynamics for carbon dioxide and an enhancement for neutral methane gas molecules [3].

[1] S.Y. Buhmann, Dispersion forces 1, Springer Heidelberg (2012).

[2] J. Fiedler et al., Effective Polarizability models, J. Phys. Chem. A 121, 9742 (2017).

[3] J. Fiedler et al., Impact of effective polarisability models on the predicted release dynamics of CH₄ and CO₂ from premelted ice, submitted (2018).