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CO2 capture in amine solutions from ab initio molecular dynamics[1] CHANGRU MA, FABIO PIETRUCCI, WANDA ANDREONI, Swiss Federal Institute of Technology Lausanne, Switzerland — The most mature technology for post-combustion CO_2 capture exploits a cyclic process, in which CO_2 is selectively and reversibly absorbed in an amine solution, typically monoethanolamine(MEA) at 30%wt concentration. Empirical efforts are ongoing worldwide to reduce the high energy penalty for amine regeneration and to increase the absorption rate. Computer simulations can help by providing new insights and the missing quantitative information. Using extensive large-scale Car-Parrinello molecular dynamics simulations, aided by accelerated sampling techniques, we have characterized the reactions leading to CO_2 capture in MEA 30%wt solutions via the formation of the carbamate, and the subsequent CO_2 release. Deprotonation and CO_2 release turn out to be competitive for an intermediate zwitterion (free-energy barrier $\sim$10kcal/mol), with sizable entropic contribution, whereas CO_2 release from the carbamate has a much higher barrier ($\sim$50kcal/mol), mainly enthalpic and rather independent of temperature. An unprecedented characterization of structural and vibrational properties of the solution allows us to interpret recent experimental results. More results on other amines, allow us to rationalize their still unexplained better performance relative to MEA.

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Wanda Andreoni
Swiss Federal Institute of Technology Lausanne

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