CO_2 capture for energy harvesting: atomistic modelling of the working mechanism

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It is well known that industrial process by-products pose a great threat for the environment. Among them, CO_2 is considered one of the most harmful because of its role in the formation of the greenhouse effect. CO_2 release in the atmosphere can be avoided by exploiting the so-called carbon capture, the process of sequestration of CO_2 thanks to a chemical reaction with a more stable compound. The technologies so far employed for capturing CO_2 are limited to the only selective capture and release of harmful gas, so they do not involve any form of energy recovery. Our research group has recently developed a new device able to harvest energy while absorbing CO_2, exploiting a supercapacitor setup in which an ionic liquid (IL) is both the electrolyte and the capturing agent. Through one of the two electrodes, CO_2 gas is fluxed when the device is in open circuit. The portion of the IL in proximity of the electrode captures the CO_2 while, on the other side of the device at the counter electrode, the IL remains unchanged. At the same time, a voltage rise is measured. Energy is, then, extracted by closing the circuit and discharging the device. Because the CO_2 capture of the IL is a chemical process and not an electrochemical one, the reasons of the voltage increase are still unclear. By means of classical molecular dynamics simulations, it was possible to associate the potential variation to the effect of charge redistribution in the ion of the IL induced by the capture of CO_2 and to the difference in chemical potential between the two ends of the device.