New Derived-N-Heterocyclic Olefins Compounds for CO_2 Capture: A Computational Study

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Computational quantum chemistry tools are used to design triazolylidene-derived N-heterocyclic olefins (trNHOs) compounds for CO_2 capture. DLPNO-CCSD(T) calculations reveal low barrier heights for the trNHOs-mediated process, which indicate that the tailored compounds are very promising for fast CO_2 sequestration. The presence of different substitutes at distinct N positions of the trNHO ring affects the CO_2 sequestration. Improved trNHO carboxylates for faster CO_2 capture/release are proposed.