Report on “A classical simulation study for carbon dioxide adsorption and separation capacity of MIL-53(Cr)” submitted for publication in Quy Nhon University Journal of Science.

In addition to the escalating depletion of fossil fuel-based energy sources, toxic emissions, particularly carbon dioxide (CO_2), are rapidly increasing, leading to an alarming impact on the environment and human health. Therefore, reducing or converting CO_2 into high-value chemicals is necessary. In this manuscript, aiming to explore the application potential of metal-organic frameworks (MOFs), the authors studied the capacities of CO_2 capture and CO_2/H_2 separation on MIL-53(Cr) at different temperatures and low pressures below 50 bar. They pointed out that the CO_2 adsorption capacity with and without hydrogen and CO_2/H_2 selectivity of MIL-53(Cr) are relatively high. Remarkably, the maximum CO_2/H_2 selectivity of MIL-53(Cr) is almost independent on the CO_2/H_2 mole fraction, but dramatically dependent on temperature. I find this result interesting and deserving publication in in Quy Nhon University Journal of Science, provided the following issue is addressed:

To be more consistent with the simulation results presented in section 3.1, where the CO_2 adsorption of MIL-53(Cr) at $T = 298\ K$ was investigated, perhaps the figure 5 should be rearranged as the following order: (a) $T = 298\ K$, (b) $T = 273\ K$, (c) $T = 323\ K$ and (d) $T = 348\ K$. The authors should revise the corresponding text to reflect these changes.