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Potential energy surface and kinetics of reaction between CO_2 and Iron

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Abstract: Since the industrial revolution, atmospheric carbon dioxide concentration has increased from 278 ppm to 400 ppm [1]. This rise is related to climate changes and it represents a challenge because of the importance of fossil fuels to the global economy [2]. To use CO_2 in a chemical reaction and to transform it into valuable products, such as chemicals and fuels, one must overcome its thermodynamic stability. Therefore, the search for transition metal-based catalysts is of major importance to chemistry [2]. Ideally, such catalysts should be cheap and made from abundant elements, in order to have a potential impact on CO_2 capture and transformation.
This study aims to determine the potential energy surface (PES) for the reaction between atomic iron and carbon dioxide. The PES is constructed using a functional form based on the many body expansion given in the equation 1. Two-, three-, and four-body interactions are calculated, respectively, using the MRCI-F12, CCSD(T)-F12 and MP2-F12 levels of theory.

$$V(\mathbf{R}) = \sum_a V_a^{(1)} + \sum_{ab} V_{ab}^{(2)} + \sum_{abc} V_{abc}^{(3)} + V_{abcd}^{(4)} \qquad (1)$$

Key-words: Potential energy surface, reduction of carbon dioxide, MRCI, CCSD(T).
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References:
[1] D. Archer, Clim. Change 138, 1 (2016).
[2] Sakakura, Toshiyasu, Jun-Chul Choi, and Hiroyuki Yasuda, Chem. Rev 107.6 (2007): 2365-2387.