

Ab-Initio Molecular Dynamics Investigation of CH₄/CO₂ Adsorption on Calcite: Improving the Enhanced Gas Recovery Process

Giuliano Carchini,¹ Mohammed J. Al-Marri,^{2*} Ibnelwaleed A. Hussein,^{1*} Santiago Aparicio³

¹Gas Processing Center, College of Engineering, Qatar University, P.O. Box 2713, Doha, Qatar

²Department of Chemical Engineering, College of Engineering, Qatar University, P.O. Box 2713 Doha, Qatar

³Department of Chemistry, University of Burgos, 09001 Burgos, Spain

*Corresponding Authors: Prof. I.A. Hussein, ihussein@qu.edu.qa; Dr. M.J Al-Marri, m.almarri@qu.edu.qa

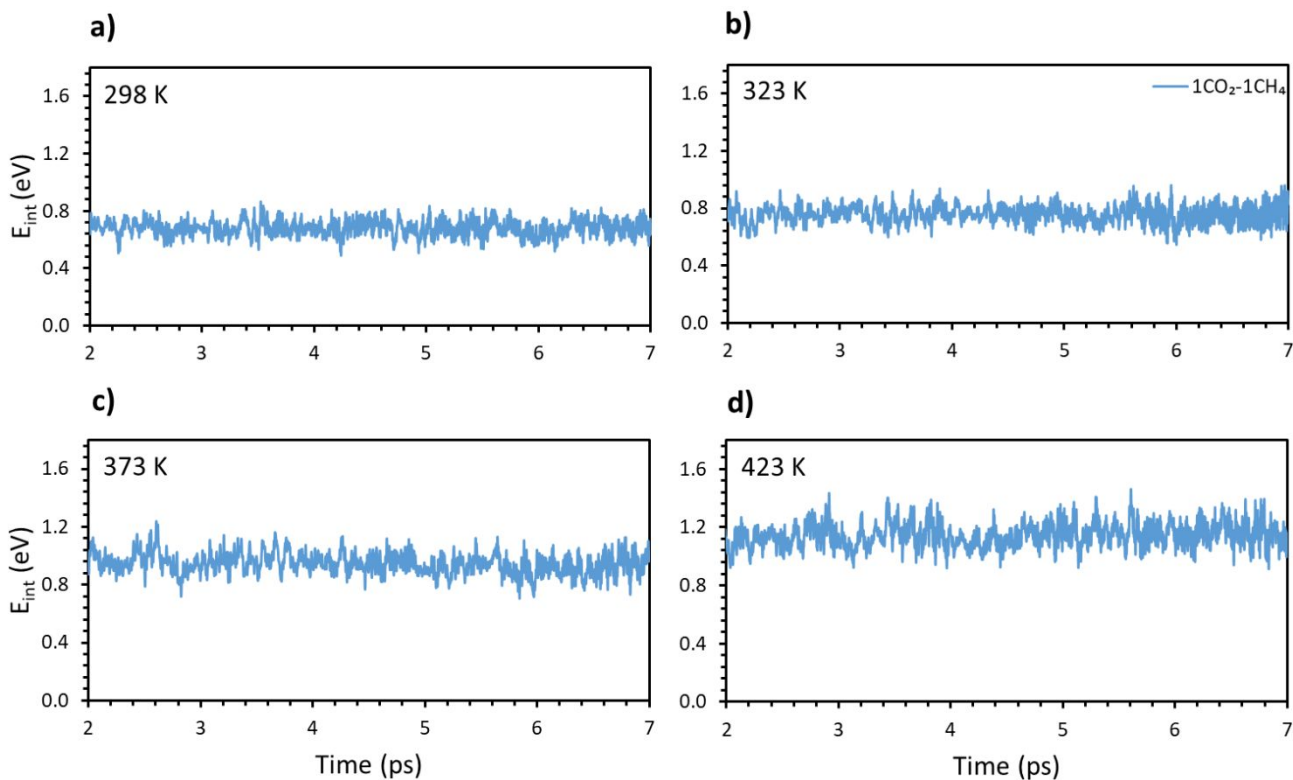


Figure S1: Interaction Energy for the mixed composition 1CO₂:1CH₄ at different temperatures: a) 298 K, b) 323 K, c) 373 and d) 423 K.

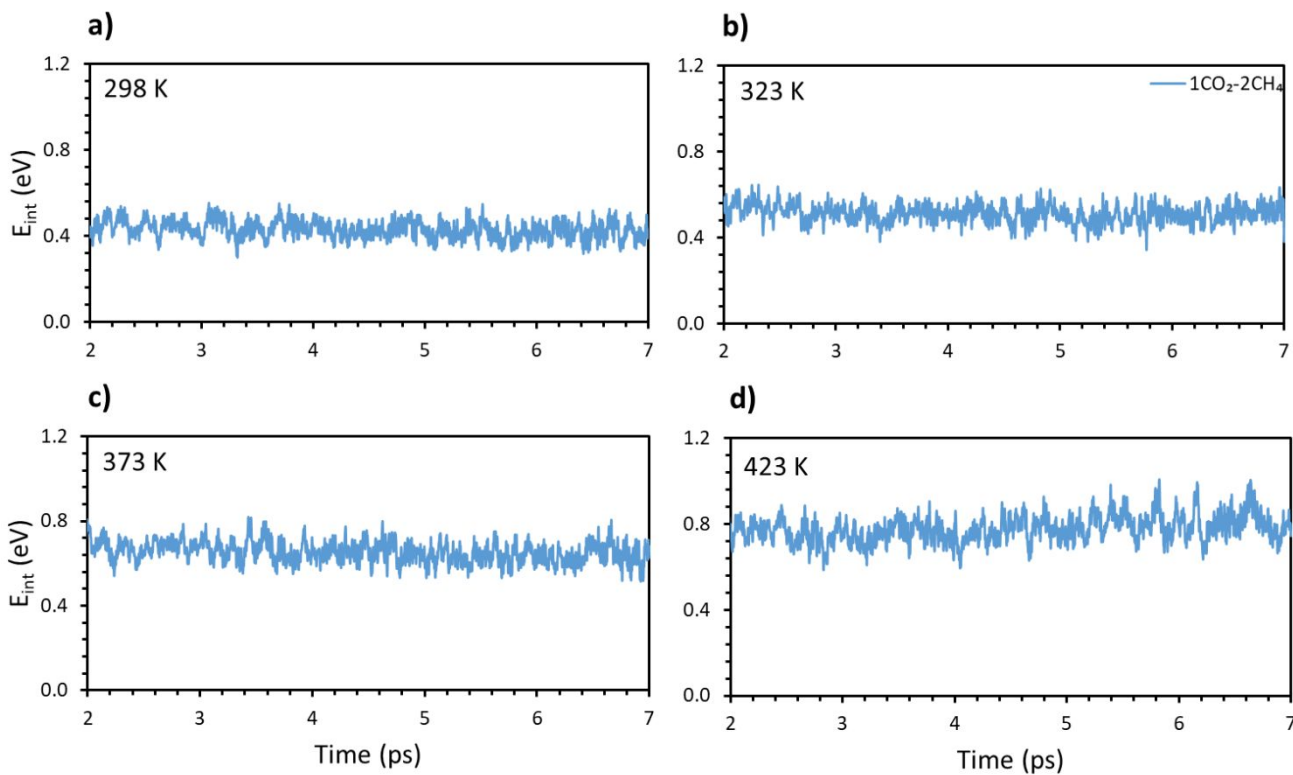


Figure S2: Interaction Energy for the mixed composition 1CO₂:2CH₄ at different temperatures: a) 298 K, b) 323 K, c) 373 and d) 423 K.

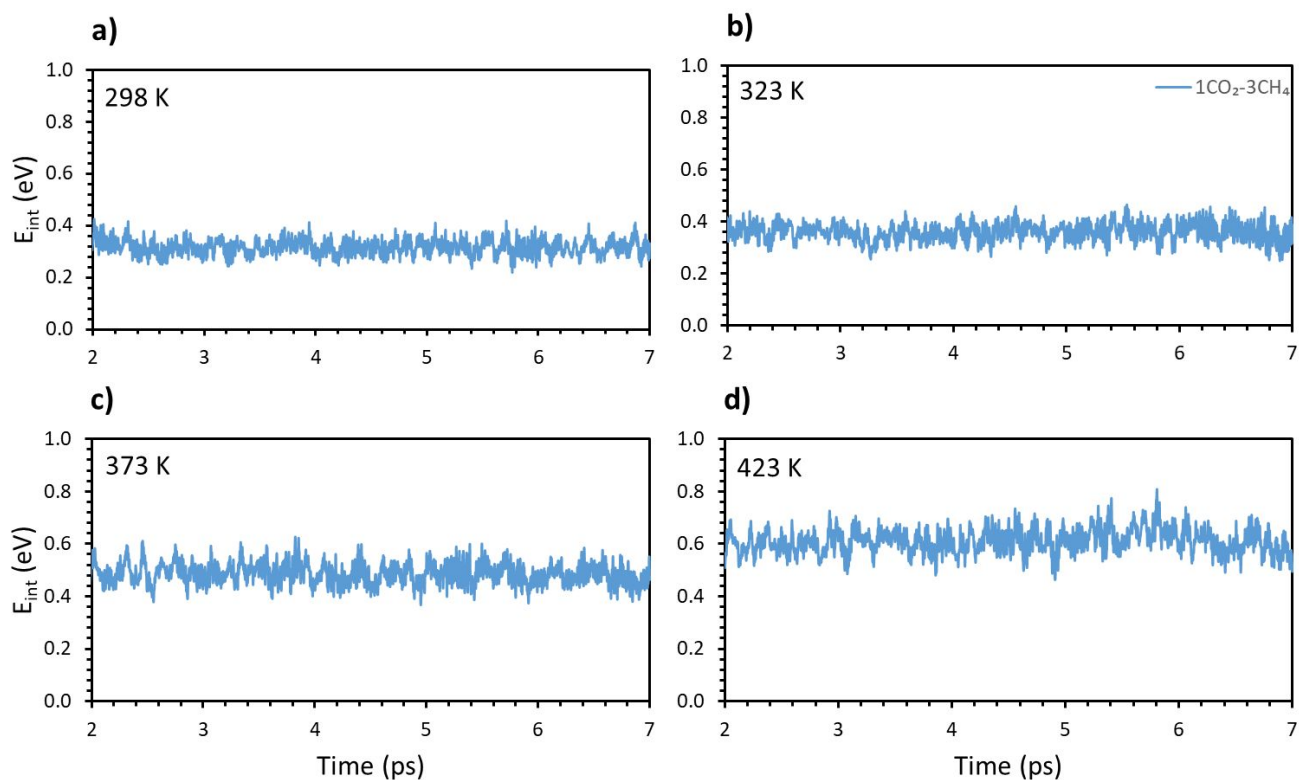


Figure S3: Interaction Energy for the mixed composition $1\text{CO}_2:3\text{CH}_4$ at different temperatures: a) 298 K, b) 323 K, c) 373 and d) 423 K.

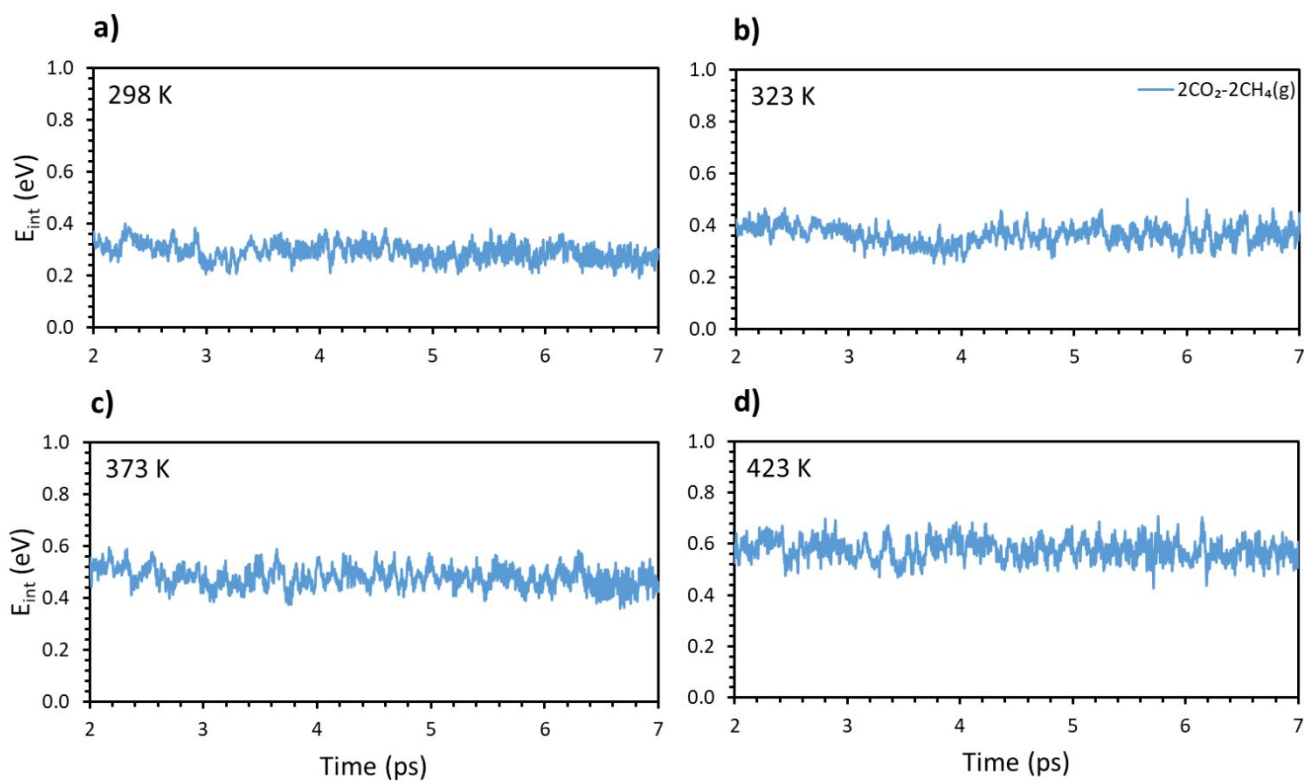


Figure S4: Interaction Energy for the gas phase $2\text{CO}_2:2\text{CH}_4$ at different temperatures: a) 298 K, b) 323 K, c) 373 and d) 423 K.