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Electronic Supplementary Information

CALCULATION OF CHEMICAL POTENTIAL AND ACTIVITY COEFFICIENT OF TWO LAYERS OF CO2 ADSORBED ON A GRAPHITE SURFACE

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S1. Average temperature and potential energy of a system with T=300K, N_{CO2}=1000 during a 2000ps of *NVE* ensemble run. Other systems with different temperatures and particle numbers (N_{CO2}) were also found to be in such stable conditions.

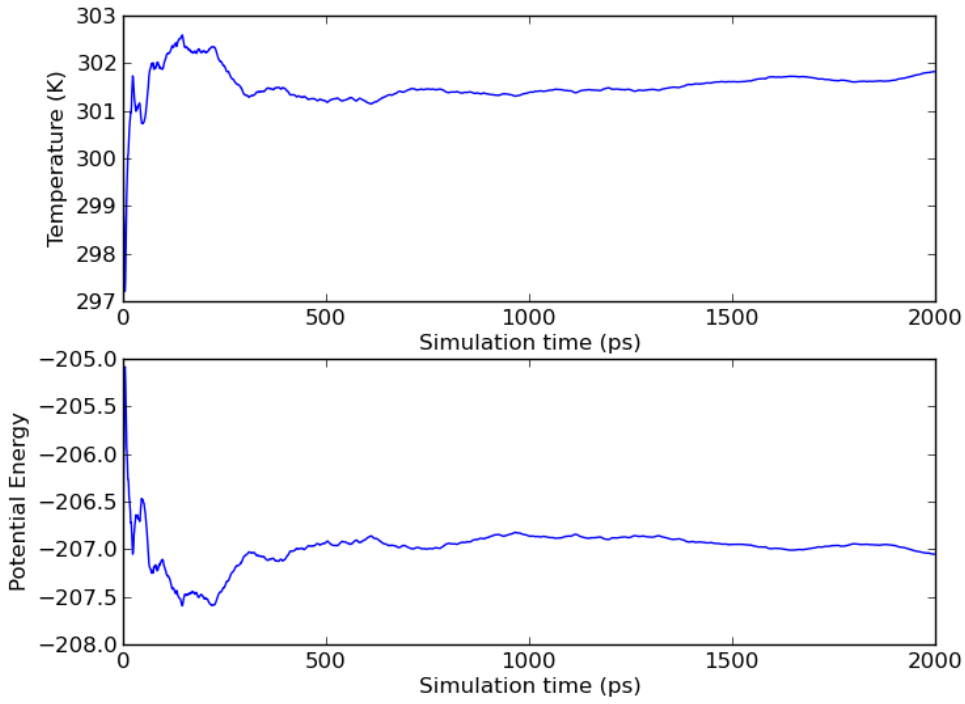

Figure S1. Average temp and potential energy of CO_2 during 2000ps run at T=300K, N_{CO2}=1000.

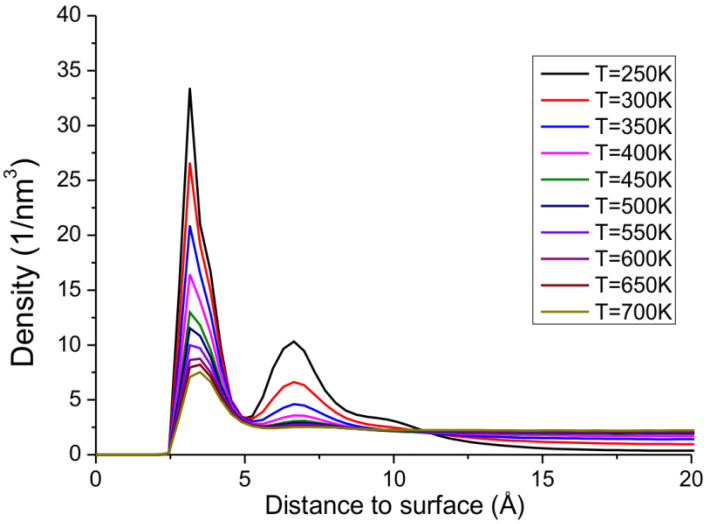

Figure S2. The density of CO_2 molecules as a function of distance to the surface, in a reservoir with N_{CO2}=2000 at temperatures between 250K -700K. At a low temperature (250K) three layers of CO_2 can be formed, and at high temperature (700K) there is only one layer of CO_2. Hence we avoided the region of too low or too high temperatures. The temperature range, 300K-550K, was chosen, in order to study two layers of adsorbed CO_2.

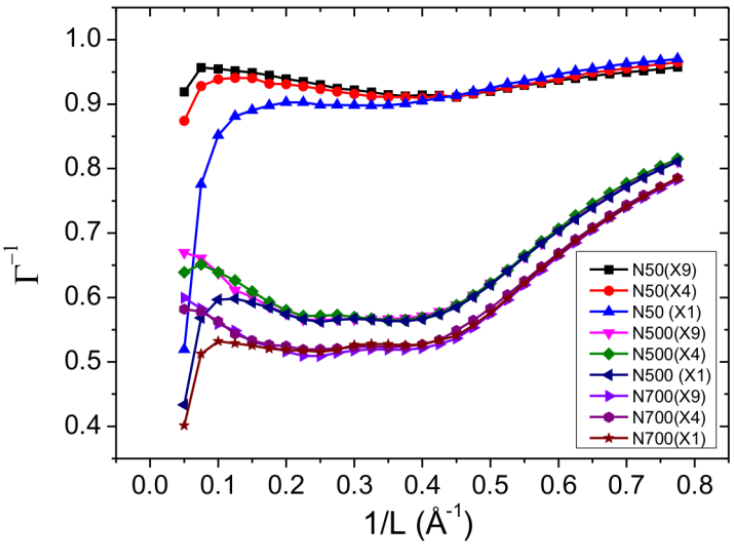

Figure S3. The impact of reservoir size on the value of Γ^{-1} of the total adsorption. Results from studies of three reservoir sizes, X1, X4 and X9, are shown studied at three densities, corresponding to N = 50, 500 and 700 molecules. Results for X4 and X9 coincide, while results for X1 deviate from these.

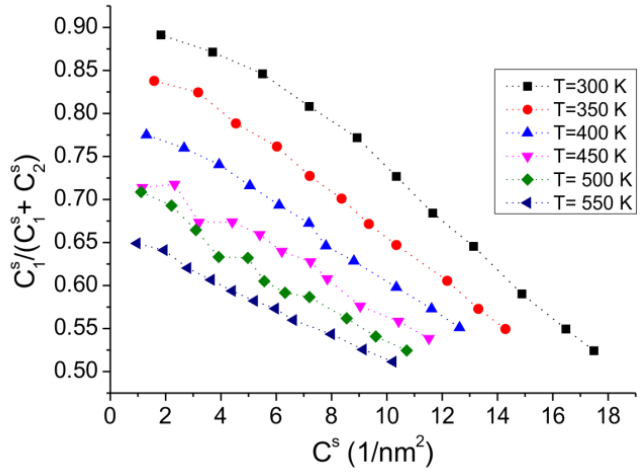

Figure S4. Fraction of molecules in the first layer as a function of the total adsorption in the temperature range 300 – 550 K.

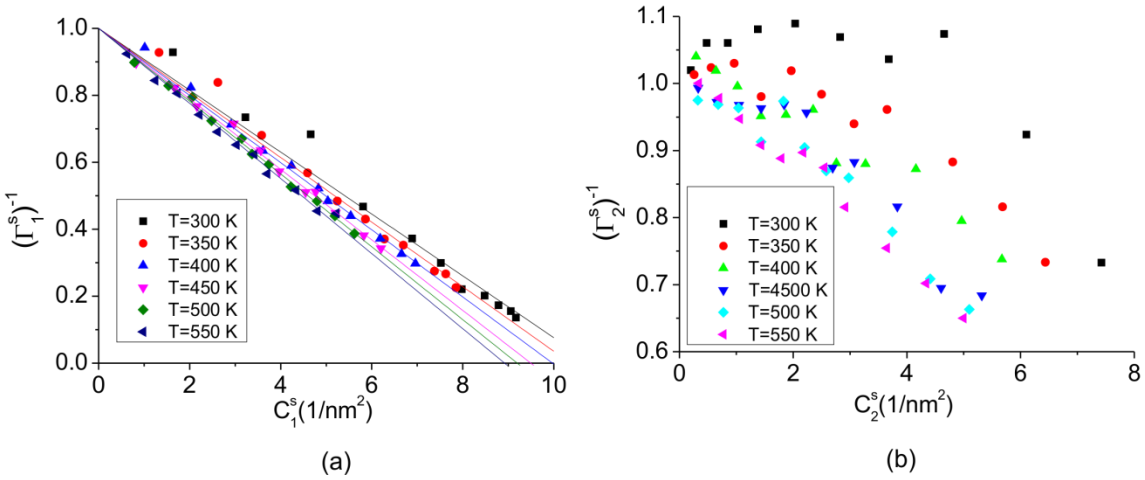

Figure S5. The inverse thermodynamic correction factor Γ^{-1} of the first (a) and second layer (b), as a function of the adsorption in the layer, at different temperatures. The first layer shows linear trends (left), while the second layer may only be fitted to a line at high temperatures.

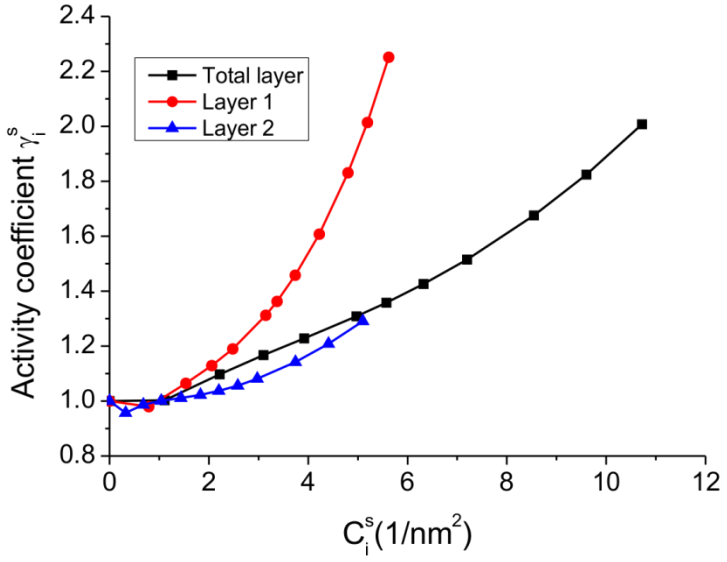

Figure S6. Activity coefficient of the first, second and the total layer as a function of the layer adsorption in the respective layer at T=500K.

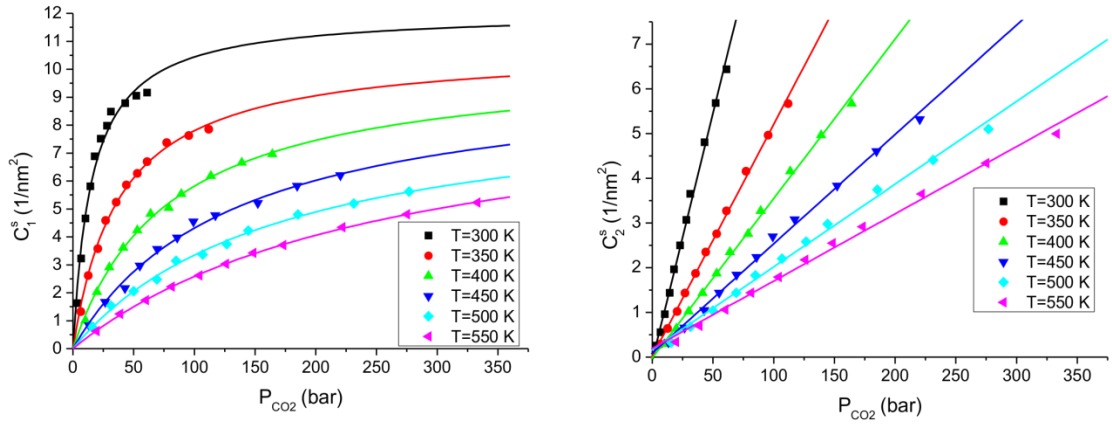

Figure S7. Adsorption isotherms for the first and second layer as function of pressure at different temperatures. The lines are fitted with the Langmuir isotherm (layer1) and with the Henry's law (layer2).