Supporting Information: Flexibility in the Graphene Sheet: The Influence on Gas Adsorption from Molecular Dynamics Studies

Jelle Vekeman,[†,‡,§] José Sánchez-Marín,[‡] Alfredo Sánchez de Merás,[*,¶]

Inmaculada Garcia Cuesta,[*,¶] and Noelia Faginas-Lago[*,†]

†*Dipartimento di Chimica, Biologia e Biotecnologie, Università degli Studi di Perugia, Via Elce di Sotto 8, I-06123 Perugia*

‡*Instituto de Ciencia Molecular, Parc cientifico de la Universidad de Valencia, C/ Catedrático José Beltrán 2, E-46980 Paterna, Spain*

¶*Departamento de Química Física, Universidad de Valencia, Avda Dr. Moliner 50, E-46100 Burjassot, Spain*

§*ALGC, Free University Brussels (VUB), Pleinlaan 2, 1050 Brussels, Belgium*

E-mail: alfredo.sanchez@uv.es; inmaculada.garcia-cuesta@uv.es; noelia.faginaslago@unipg.it

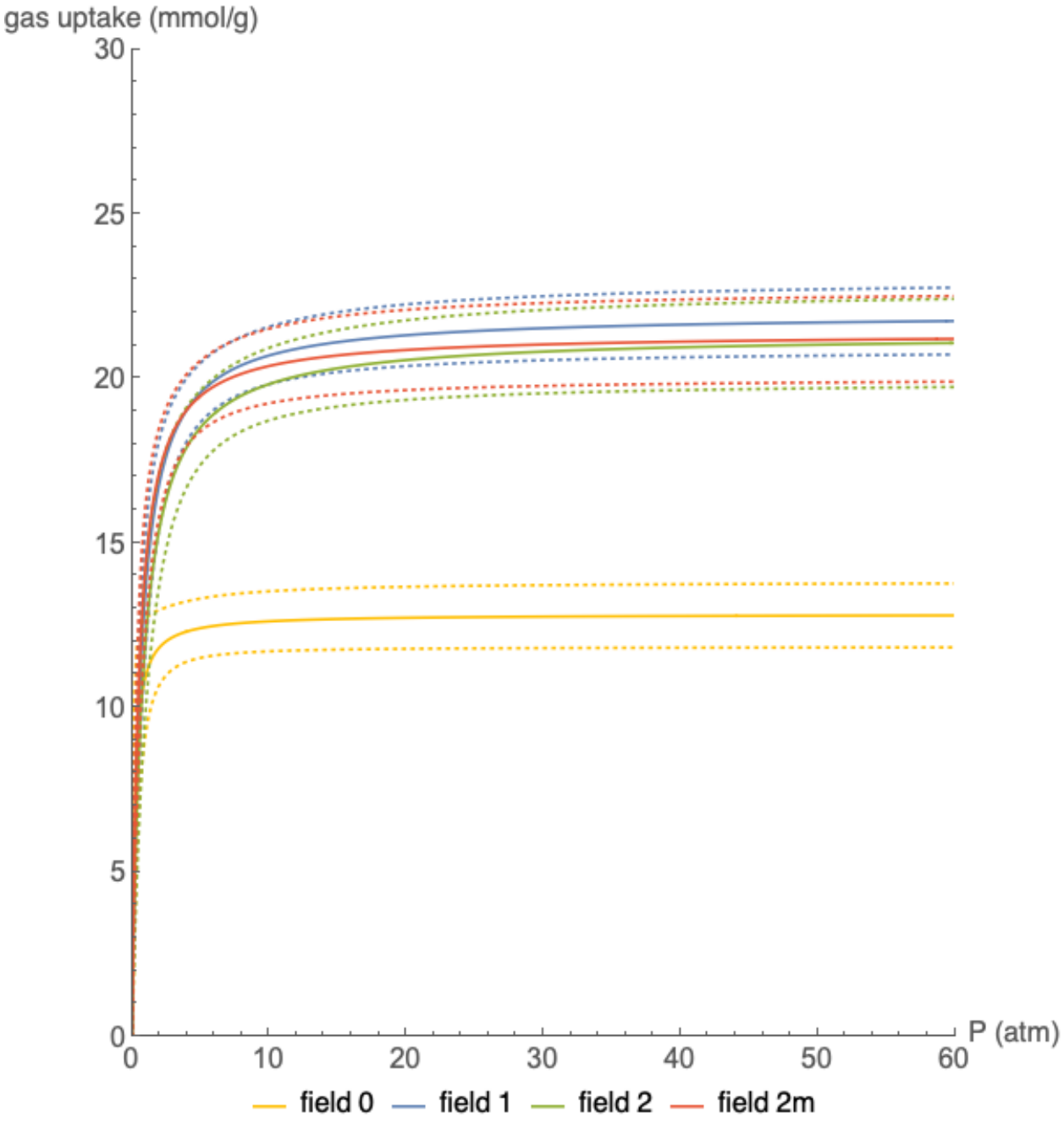

Figure S1: Comparison of methane adsorption isotherms for the four different models of the sheet and using the united-atom model for the adsorbate. Dotted lines represent 95% confidence bands of the regression analysis of the simulated data.

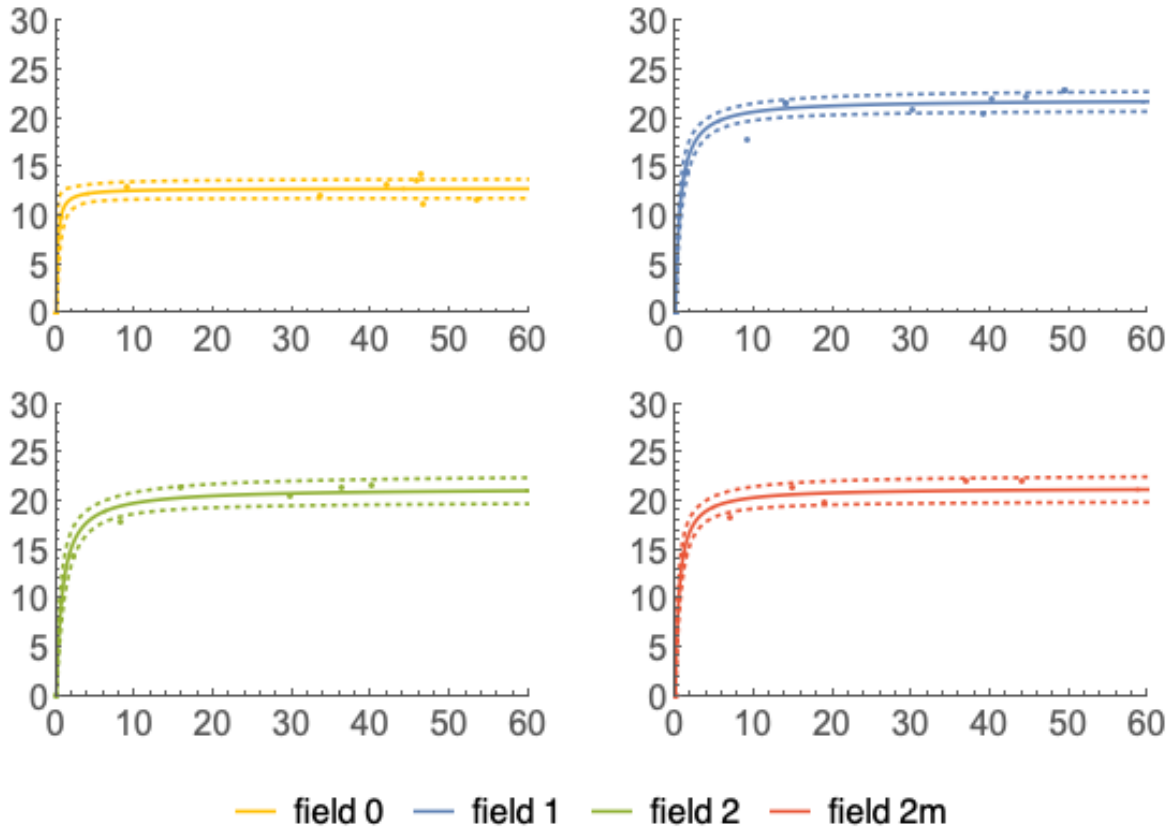

Figure S2: Methane adsorption isotherms (uptake/mmol.g-1 v.s. P/atm) in the united-atom approach, for each graphene sheet model used. Dotted lines represent 95% confidence bands. The conventions are the same as in Figure S1

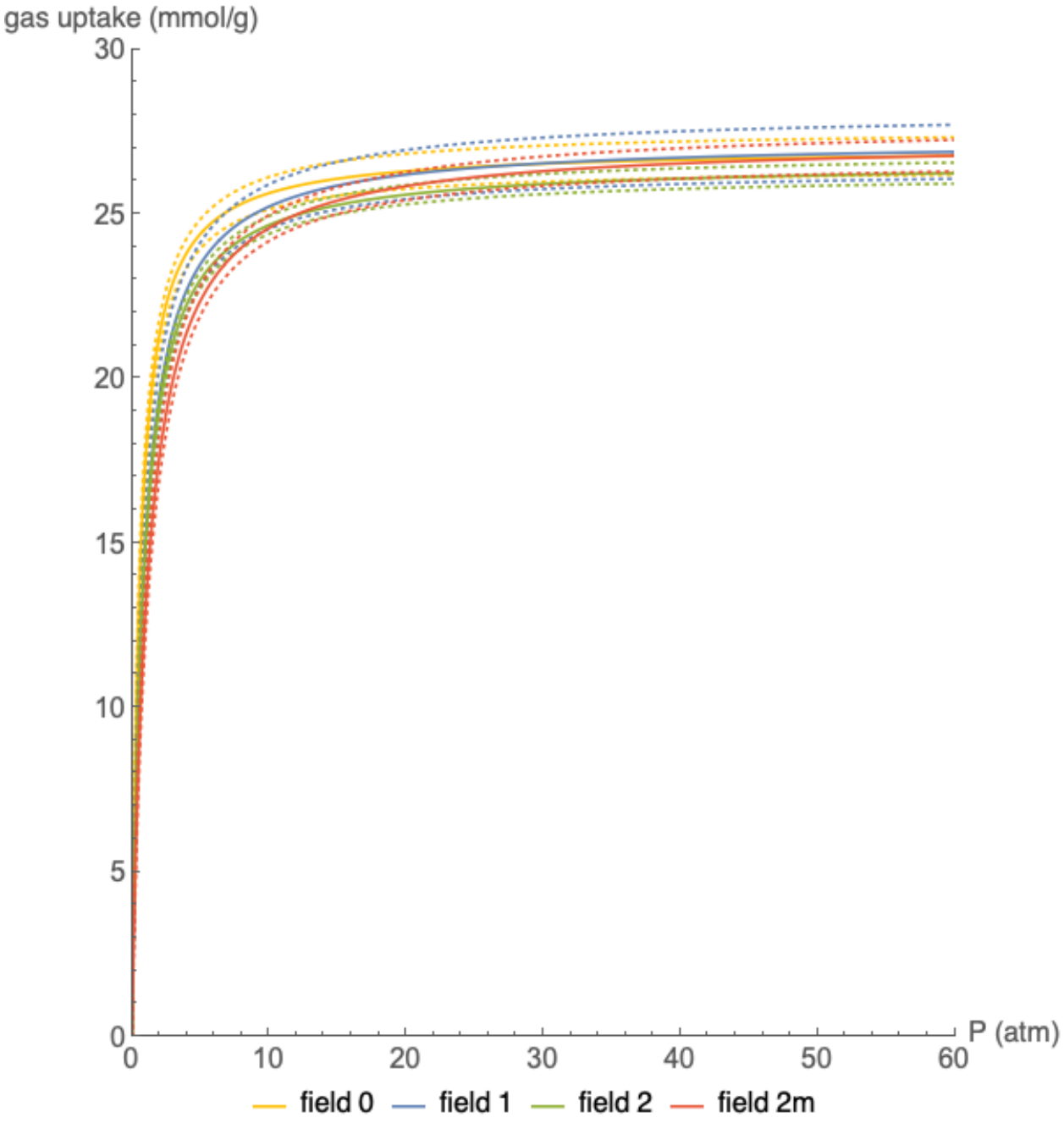

Figure S3: Comparison of methane adsorption isotherms for the four different models of the sheet and using the atomistic model for the adsorbate. Dotted lines represent 95% confidence bands of the regression analysis of the simulated data.

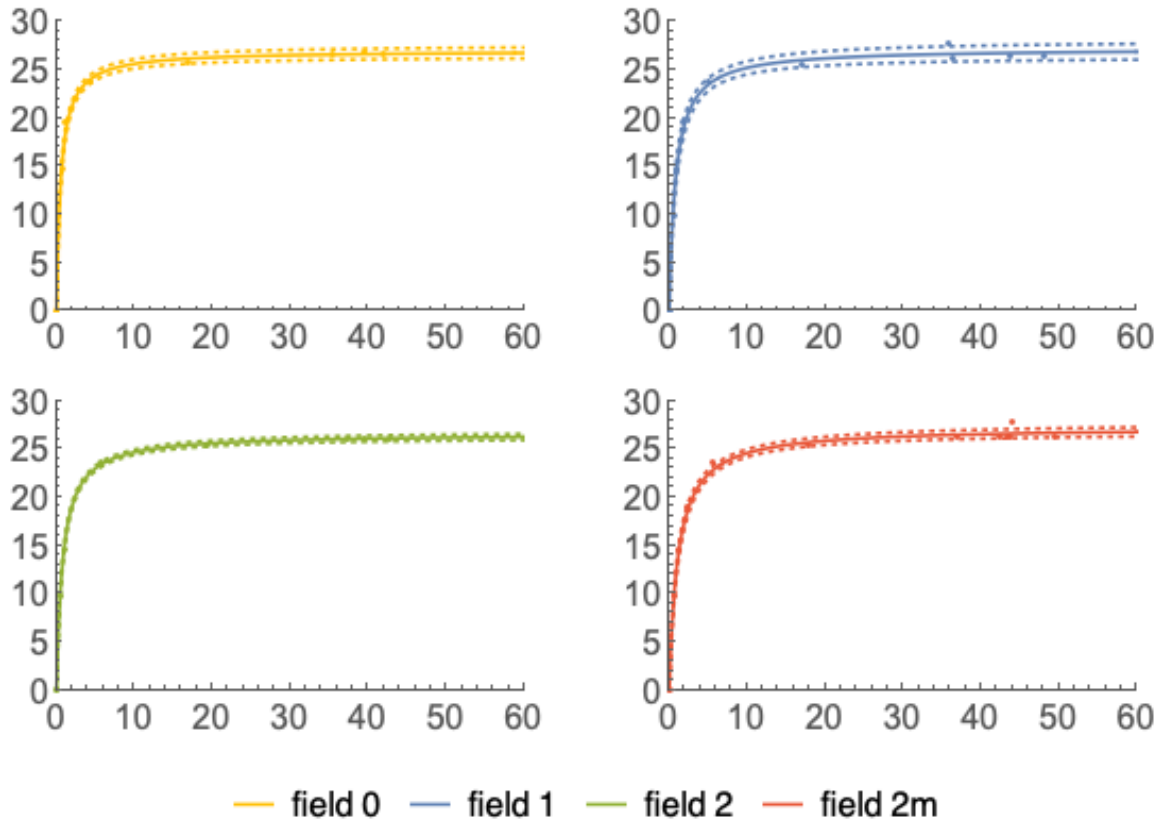

Figure S4: Methane adsorption isotherms (uptake/mmol.g-1 v.s. P/atm) in the atomistic approach, for each graphene sheet model used. Dotted lines represent 95% confidence bands. The conventions are the same as in Figure S1

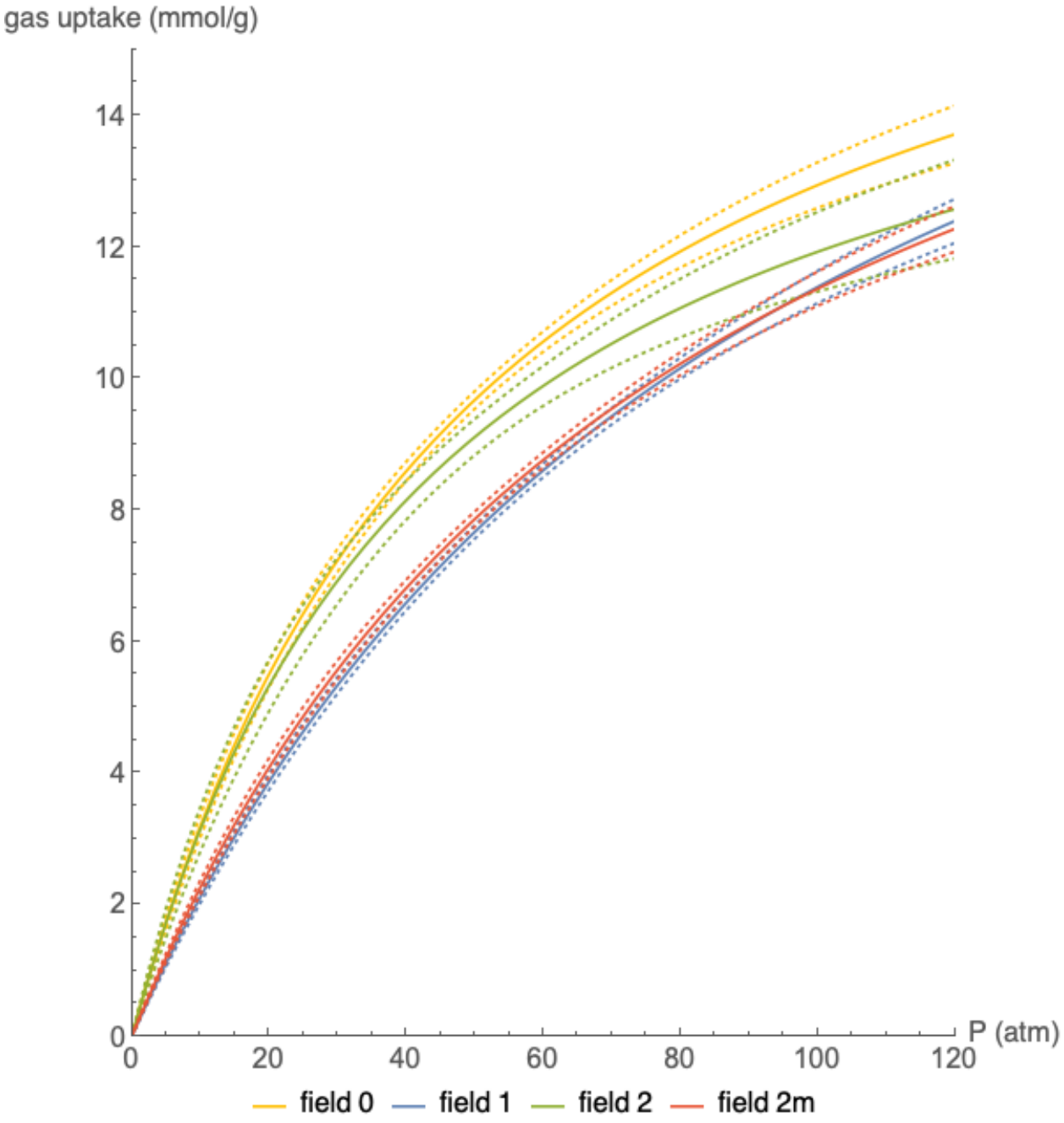

Figure S5: Comparison of nitrogen adsorption isotherms for the four different models of the sheet and using the united-atom model for the adsorbate. Dotted lines represent 95% confidence bands of the regression analysis of the simulated data.

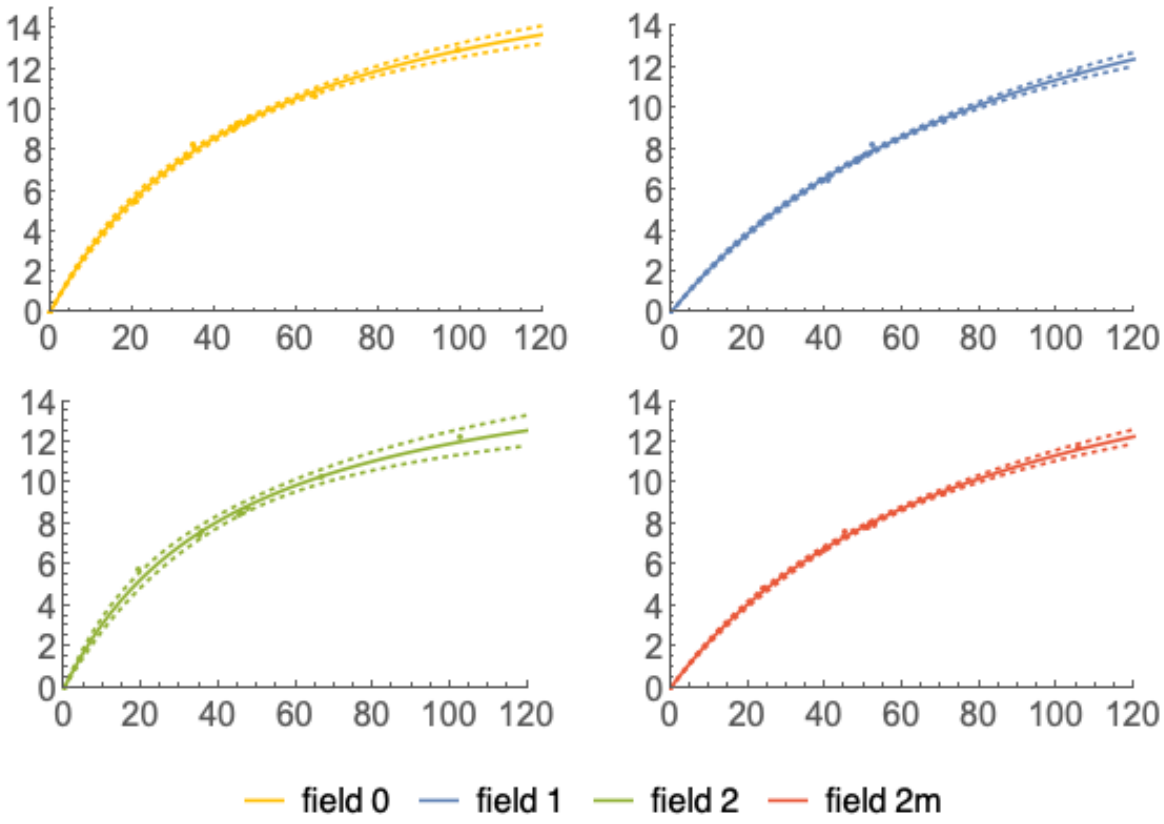

Figure S6: Nitrogen adsorption isotherms (uptake/mmol.g-1 v.s. P/atm) in the united-atom approach, for each graphene sheet model used. Dotted lines represent 95% confidence bands. The conventions are the same as in Figure S1

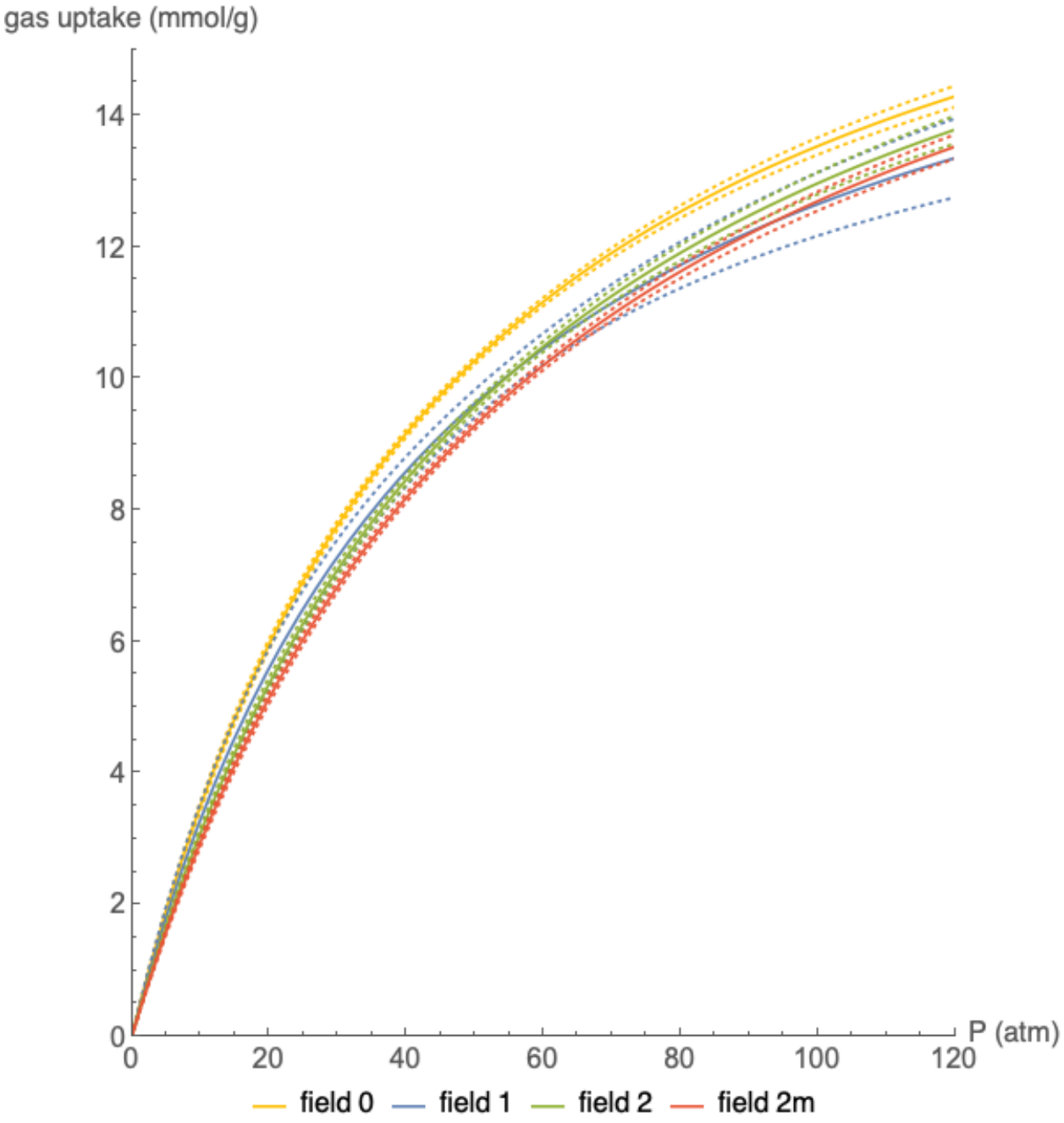

Figure S7: Comparison of nitrogen adsorption isotherms for the four different models of the sheet and using the atomistic model for the adsorbate. Dotted lines represent 95% confidence bands of the regression analysis of the simulated data.

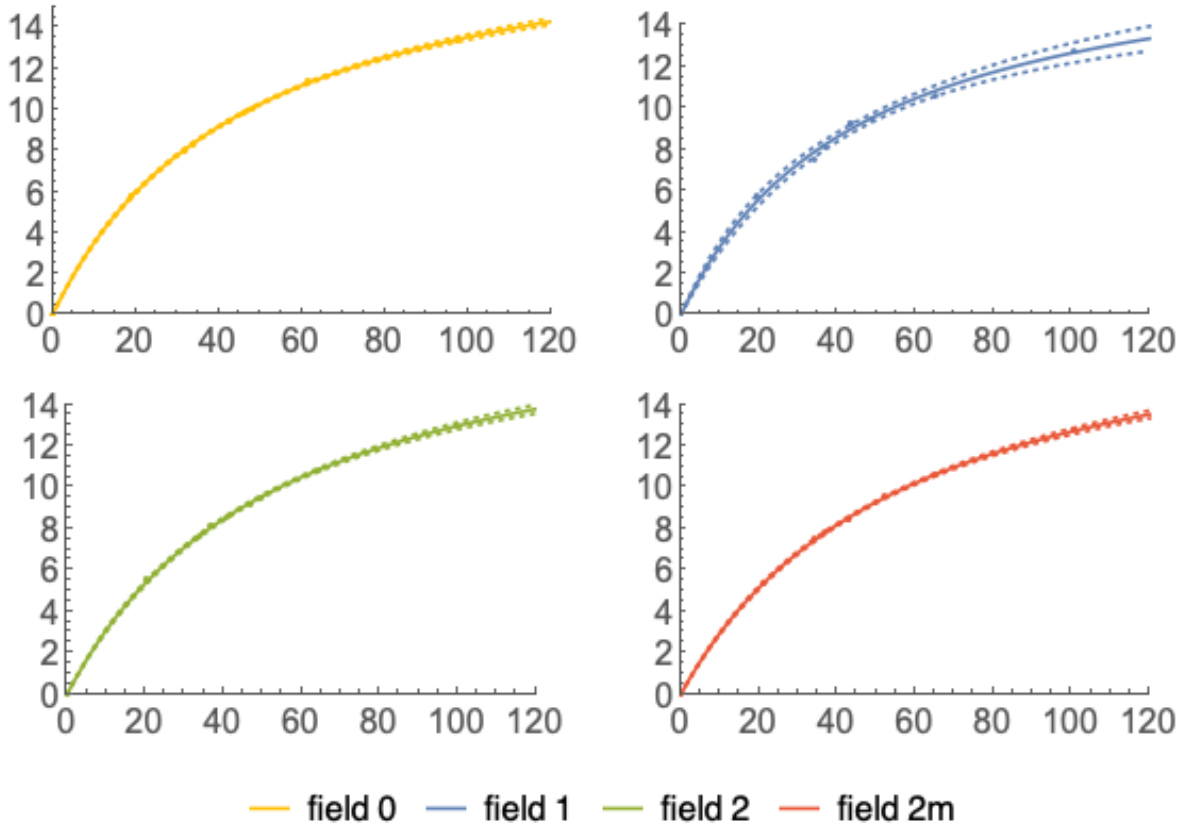

Figure S8: Nitrogen adsorption isotherms (uptake/mmol.g-1 v.s. P/atm) in the atomistic approach, for each graphene sheet model used. Dotted lines represent 95% confidence bands. The conventions are the same as in Figure S1