Universidad de Valparaíso
CHILE
Doctorado en Ciencias mención Biofísica y Biología Computacional

CENTRO INTERDISCIPLINARIO DE Neurociencia de Valparaíso

Thermodynamic properties of amino acid adsorption over graphene

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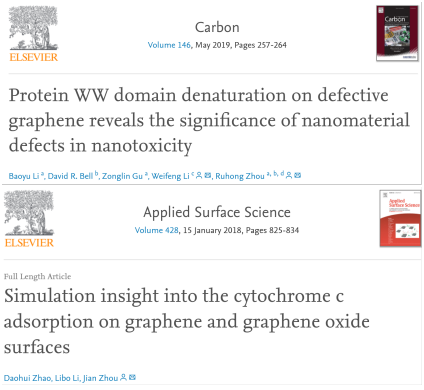
Doctorado en Ciencias mención Biofísica y Biología Computacional
2021

Studies on adsorption processes on graphene



ELSEVIER

Carbon

Volume 146, May 2019, Pages 257-264

Protein WW domain denaturation on defective graphene reveals the significance of nanomaterial defects in nanotoxicity

Baoyu Li [a], David R. Bell [b], Zonglin Gu [a], Weifeng Li [c], Ruhong Zhou [a, b, d]

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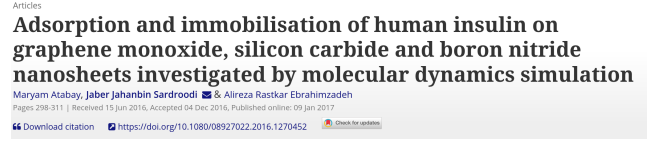
Applied Surface Science

Volume 428, 15 January 2018, Pages 825-834

Full Length Article

Simulation insight into the cytochrome c adsorption on graphene and graphene oxide surfaces

Daohui Zhao, Libo Li, Jian Zhou



Articles

Adsorption and immobilisation of human insulin on graphene monoxide, silicon carbide and boron nitride nanosheets investigated by molecular dynamics simulation

Maryam Atabay, **Jaber Jahanbin Sardroodi** & Alireza Rastkar Ebrahimzadeh

Pages 298-311 | Received 15 Jun 2016, Accepted 04 Dec 2016, Published online: 09 Jan 2017

Download citation https://doi.org/10.1080/08927022.2016.1270452 Check for updates

Reduced Cytotoxicity of Graphene Nanosheets Mediated by Blood-Protein Coating

Yu Chong[†], Cuicui Ge[†], Zaixing Yang[†], Jose Antonio Garate[‡], Zonglin Gu[†], Jeffrey K. Weber[‡], Jiajia Liu[†], and Ruhong Zhou[*†‡§]

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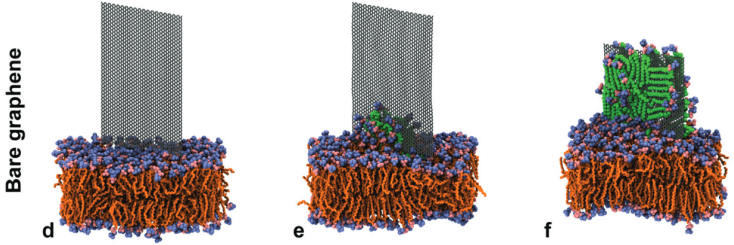
Graphene can wreak havoc in cell membranes



Issue 37, 2015

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From the journal:
Nanoscale

Protein corona mitigates the cytotoxicity of graphene oxide by reducing its physical interaction with cell membrane†

Check for updates

Guangxin Duan,‡[a] Seung-gu Kang,‡[b] Xin Tian,[a] Jose Antonio Garate,[b] Lin Zhao,[a] Cuicui Ge*[a] and Ruhong Zhou*[abc]

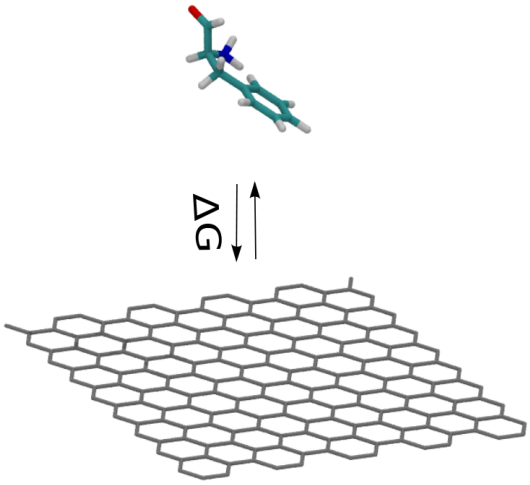
However...

- There is a lack of descriptions based on amino acid composition.
- There is a lack of rigorous thermodynamic descriptions of adsorption processes on graphene.

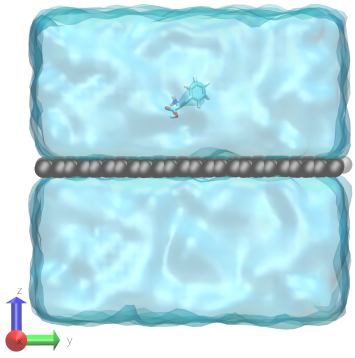
Simulations

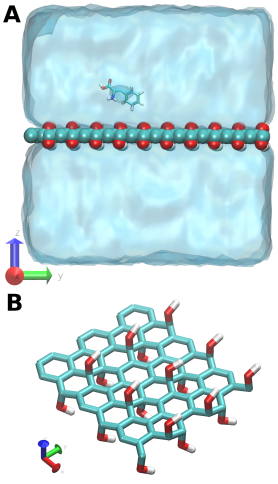
Free Energy of Adsorption

- All proteinogenic amino acids are being studied.
- ξ is defined as the distance between $\mathbf{q}_{\alpha-\text{carbon}}$ and COM(graphene), times (dot product) $(0, 0, 1)$.
- $\Delta A_{ads} = A^{adsorbed} - A^{free}$
- ΔA_{ads} was calculated using GROMOS with the umbrella sampling method.



Simulated Systems





Free Energy, Energy, and Entropy

$$\Delta A_{ads} = \langle A \rangle_{adsorbed} - \langle A \rangle_{free}$$

$$\langle A \rangle_{ab} = \frac{\sum_{i=a}^{b} A(\xi_i) p(\xi_i)}{\sum_{i=a}^{b} p(\xi_i)}$$

$$p(\xi_i) = \frac{e^{-\beta \mathrm{PMF}(\xi_i)}}{\sum e^{-\beta \mathrm{PMF}(\xi)}}$$

$$\Delta E_{ads} = \langle E \rangle_{adsorbed} - \langle E \rangle_{free}$$

$$T\Delta S_{ads} = \Delta E_{ads} - \Delta A_{ads}$$

Computing other properties

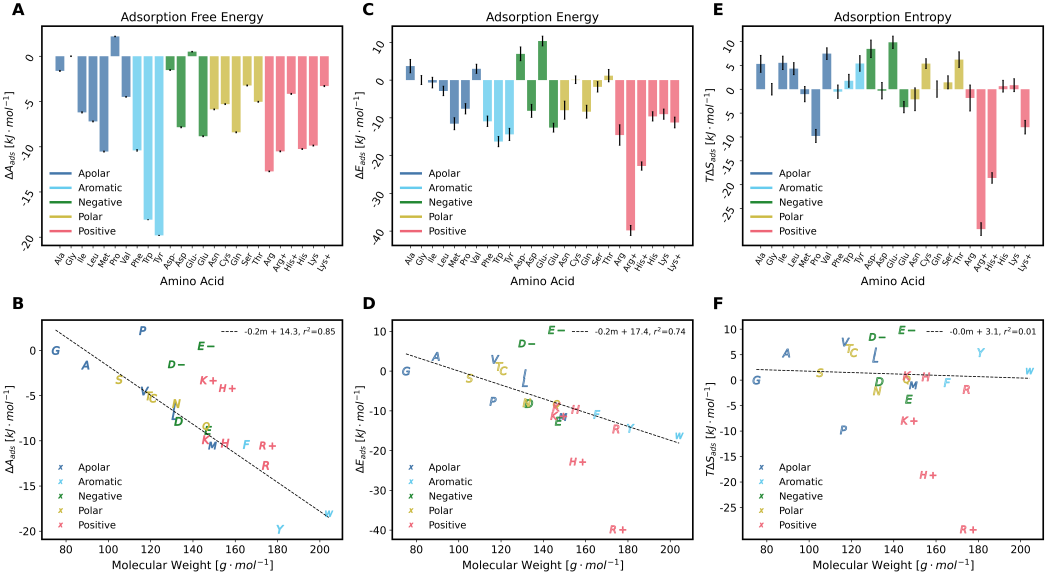
$$\langle T(\xi) \rangle = \frac{\sum_{i=1}^{M} \sum_{j=1}^{N_i} T_{i,j} e^{-\beta(A_i - V_{bias})} \delta\xi_{i,j}}{\sum_{i=1}^{M} \sum_{j=1}^{N_i} e^{-\beta(A_i - V_{bias})} \delta\xi_{i,j}}$$

ΔA^{ads}, ΔE^{ads}, $T\Delta S^{ads}$

Amino acid	ΔA	ΔE	$T\Delta S$
Alanine	-10.3 ± 0.1	-12.5 ± 1.8	-2.2 ± 1.8
Arginine	-21.4 ± 0.0	-30.7 ± 2.7	-9.3 ± 2.7
Arginine (+)	-19.2 ± 0.1	-56.0 ± 1.3	-36.8 ± 1.3
Asparagine	-14.5 ± 0.0	-24.1 ± 2.4	-9.6 ± 2.4
Aspartic Acid (-)	-10.2 ± 0.1	-9.2 ± 1.8	1.0 ± 1.8
Aspartic Acid	-16.5 ± 0.1	-24.3 ± 1.7	-7.8 ± 1.7
Cysteine	-14.0 ± 0.1	-16.1 ± 1.0	-2.1 ± 1.0
Glutamic Acid (-)	-8.2 ± 0.0	-5.8 ± 1.3	2.3 ± 1.3
Glutamic Acid	-17.5 ± 0.1	-28.8 ± 1.2	-11.3 ± 1.2
Glutamine	-17.1 ± 0.1	-24.5 ± 1.7	-7.5 ± 1.7
Glycine	-8.7 ± 0.0	-16.2 ± 1.2	-7.5 ± 1.2
Histidine (+)	-12.8 ± 0.1	-38.9 ± 1.1	-26.1 ± 1.1
Histidine	-18.9 ± 0.1	-25.8 ± 1.2	-6.9 ± 1.2

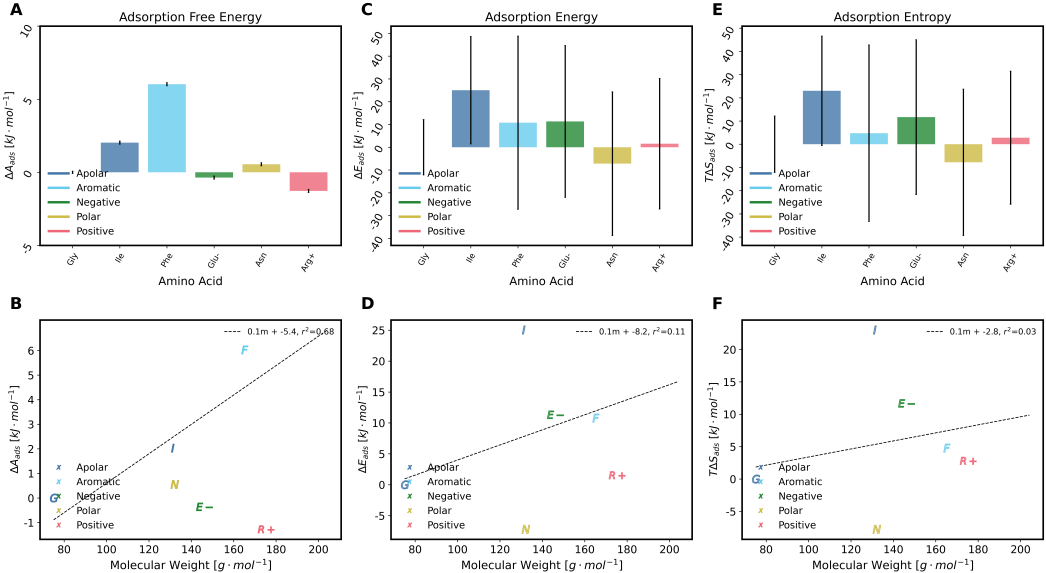
Amino acid	ΔA	ΔE	$T\Delta S$
Isoleucine	-14.9 ± 0.1	-16.8 ± 1.4	-2.0 ± 1.4
Leucine	-15.9 ± 0.1	-19.1 ± 1.3	-3.2 ± 1.3
Lysine	-18.5 ± 0.1	-25.2 ± 1.4	-6.7 ± 1.4
Lysine (+)	-12.0 ± 0.1	-27.4 ± 1.4	-15.5 ± 1.4
Methionine	-19.2 ± 0.1	-27.7 ± 1.6	-8.5 ± 1.6
Phenylalanine	-19.1 ± 0.1	-27.1 ± 1.4	-8.0 ± 1.4
Proline	-6.5 ± 0.0	-23.8 ± 1.4	-17.3 ± 1.4
Serine	-11.9 ± 0.1	-18.0 ± 1.4	-6.1 ± 1.4
Threonine	-13.7 ± 0.1	-15.0 ± 1.6	-1.3 ± 1.6
Tryptophan	-26.7 ± 0.0	-32.5 ± 1.4	-5.7 ± 1.4
Tyrosine	-28.5 ± 0.0	-30.6 ± 1.6	-2.1 ± 1.6
Valine	-13.2 ± 0.0	-13.2 ± 1.2	0.0 ± 1.2

Adsorption over Pristine Graphene



Amino acid	ΔA	ΔE	$T\Delta S$
Arginine (+)	-5.4 ± 0.1	-11.0 ± 28.7	-5.5 ± 28.7
Asparagine	-3.6 ± 0.1	-19.7 ± 31.5	-16.1 ± 31.5
Glutamic Acid (-)	-4.5 ± 0.1	-1.2 ± 33.3	3.3 ± 33.3
Glycine	-4.2 ± 0.1	-12.5 ± 12.2	-8.4 ± 12.2
Isoleucine	-2.1 ± 0.1	12.5 ± 23.6	14.7 ± 23.6
Phenylalanine	1.9 ± 0.1	-1.7 ± 38.0	-3.6 ± 38.0

Adsorption over Oxidized Graphene



Adsorption of Penta-Alanine over pristine graphene

Alanine	ΔA^{ads}	ΔE^{ads}	$T\Delta S^{ads}$
Mono	-10.3 ± 0.1	-12.5 ± 1.8	-2.2 ± 1.8
Penta (Prediction)	-43.3 ± 0.4	-52.5 ± 7.6	-9.24 ± 7.6
Penta (Stretched)	-40.4 ± 0.1	-48.8 ± 6.7	-8.4 ± 6.7
Penta (Helix)	-6.3 ± 0.1	-32.6 ± 5.4	-26.2 ± 5.5