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Author Name

- Mills, R. (12)
- Busch, P. (3)
- Gell-Mann, M. (3)
- Man'ko, V.I. (3)
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| | | | | | |
|--------------------------|---|-----------------------------|------|---|------------|
| <input type="checkbox"/> |  Quantum mechanics, high energy physics and accelerators: Selected papers of John bell | [No author name available] | 1990 | World Scientific pp. 221-233 | 1 |
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| <input type="radio"/> Conference Paper | (881) |
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Autores especialistas, experts.

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| <input type="radio"/> Physical Review B Condensed Matter and Materials Physics | (1,632) |
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
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- Quantum mechanics studies of cellobiose conformations

French, A.D., Johnson, G.P.

2006 Canadian Journal of Chemistry
84 (4), pp. 603-612

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| <input type="checkbox"/> 1 | Prediction of potency of protease inhibitors using free energy simulations with polarizable quantum mechanics-based ligand charges and a hybrid water model | Das, D., Koh, Y., Tojo, Y., Ghosh, A.K., Mitsuya, H. | 2009 | Journal of Chemical Information and Modeling | 14 |
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- Karabacak, M. (37)
- Truhlar, D.G. (35)
- Tunon, I. (34)

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- Chemistry (2,983)
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Journal of Molecular Structure: THEOCHEM

Volume 946, Issue 1-3, 30 April 2010, Pages 26-32

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Electron binding energies of free base porphyrin and magnesium-porphyrin: A sequential Born-Oppenheimer molecular dynamics/quantum mechanics approach (Article)


Martinião, H.F.M.C.^a, Cabral, B.J.C.^{ab}  ^a Grupo de Física Matemática, Universidade de Lisboa, Av. Professor Gama Pinto 2, 1649-003 Lisboa, Portugal^b Departamento de Química e Bioquímica, Faculdade de Ciências, Universidade de Lisboa, 1749-016 Lisboa, Portugal

[Ionization of chlorophyll-c 2 in liquid methanol](#)
Jaramillo, P., Coutinho, K., Cabral, B.J.C.
(2012) Chemical Physics Letters

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Abstract

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The electronic properties of free base porphyrin (H₂P) and magnesium-porphyrin (MgP) were investigated through a sequential Born-Oppenheimer molecular dynamics/quantum mechanics approach. The quantum mechanics calculations for the electronic density of states were performed with Green's function or electron propagator theory and also with a recent series of approximations for the exchange-correlation functional proposed by Truhlar and collaborators. The distortions of the porphyrin structures were analysed through normal-coordinate structural decomposition. The role played by thermal effects on structural distortions of H₂P and MgP and their relationship with electron binding energies are discussed. Our results indicate that distortions of the porphyrin macrocycle induced by thermal effects do not influence in a significant way electron binding energies for the valence states of H₂P and MgP. However, some correlation has been observed between nonplanar breathing distortions and electron binding energies of Mn(1s), Mn(2s), and Mn(2p) states, which can be blue-shifted by ~0.8

Related documents

[Ab initio electron propagator calculations on the ionization energies of free base porphine, magnesium porphyrin, and zinc porphyrin](#)
Dolgounitcheva, O., Zakrzewski, V.G., Ortiz, J.V.
(2005) Journal of Physical Chemistry A

[Density functional theory for transition metals and transition metal chemistry](#)

Resumen y documento de información

report an experimental study of a condensed-matter system (graphene, a single atomic layer of carbon) in which electron transport is essentially governed by Dirac's (relativistic) equation. The charge carriers in graphene mimic relativistic particles with a small effective mass. Many unusual phenomena that are characteristic of unusual materials do not appear in this two-dimensional system. In particular, graphene's conductivity never changes from a metallic state to an insulating state at low temperatures or in magnetic fields; the carrier concentration is independent of temperature; and the carrier concentration is independent of carrier concentration at half-integer filling factors; and the carrier concentration is independent of carrier concentration in this two-dimensional system is not only interesting in itself but also allows access to the subtle and rich physics of quantum electrodynamics in a bench-top experiment. © 2005 Nature Publishing Group.

Palabras clave indexados, el número de registros de otras fuentes de la investigación y los detalles del artículo publicado

Indexed keywords

Engineering controlled terms: Electric conductance; Electric conductivity; Electrodynamics; High energy physics; Quantum electronics; Quantum theory

Engineering uncontrolled terms: Cosmology; Quantum electrodynamics; Two-dimensional system

Engineering main heading: Fermions

EMTREE drug terms: carbon

GEOBASE Subject Index: physics

EMTREE medical terms: article; conductance; electron transport; fermion; gas analysis; mathematical analysis; molecular mechanics; molecular weight; particle size; physics; priority journal; quantum mechanics

Chemicals and CAS Registry Numbers: carbon, 7440-44-0

ISSN: 00280836 CODEN: NATURE
DOI: 10.1038/nature04242

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Rose, M.E.
1 (1961) *Relativistic Electron Theory*. Cited 311 times.

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Geim, A.K. , Novoselov, K.S.
(2007) *Nature Materials*

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(2007) *Solid State Communications*

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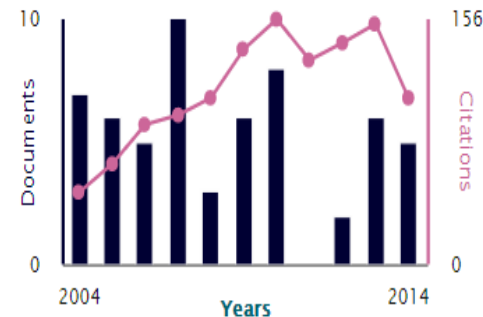
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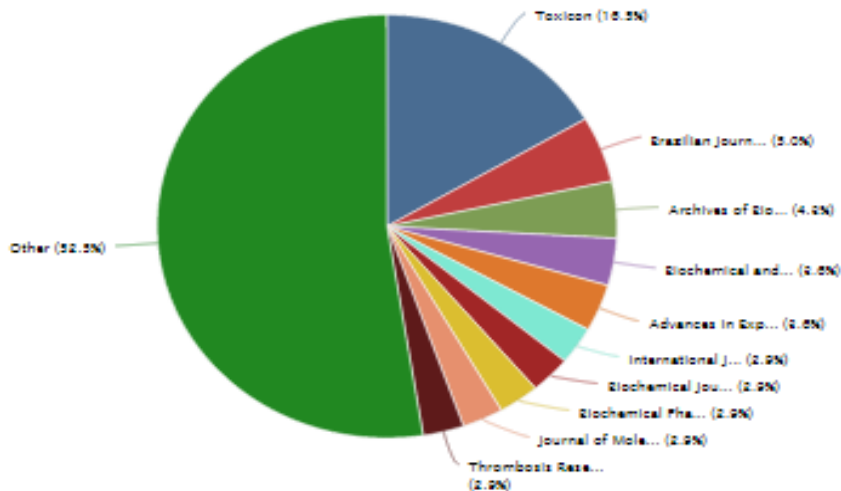
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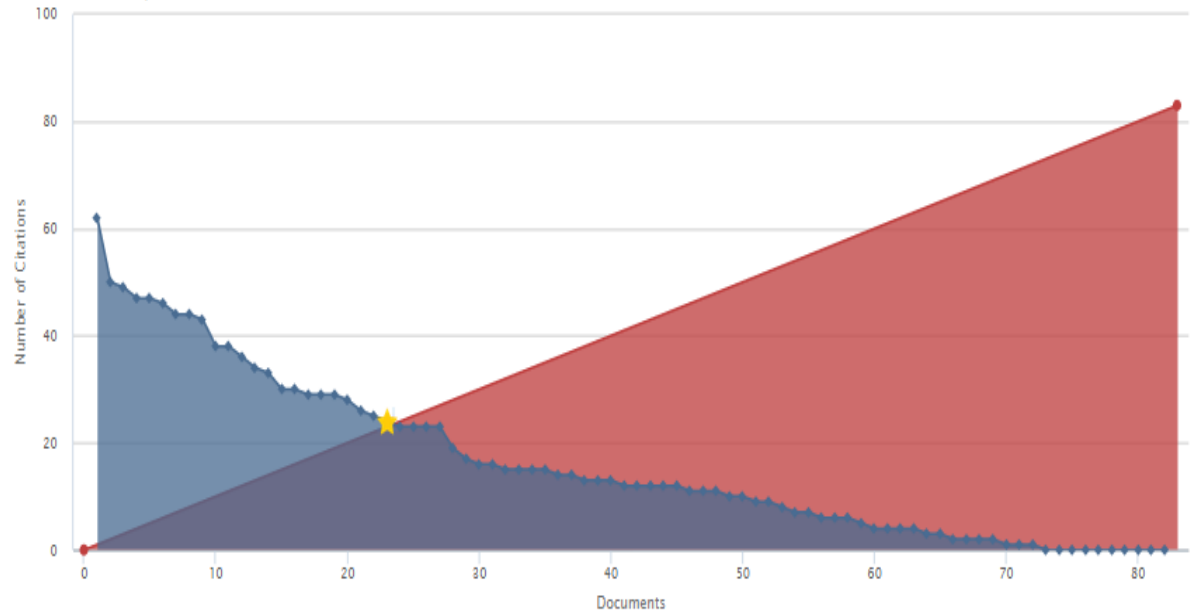
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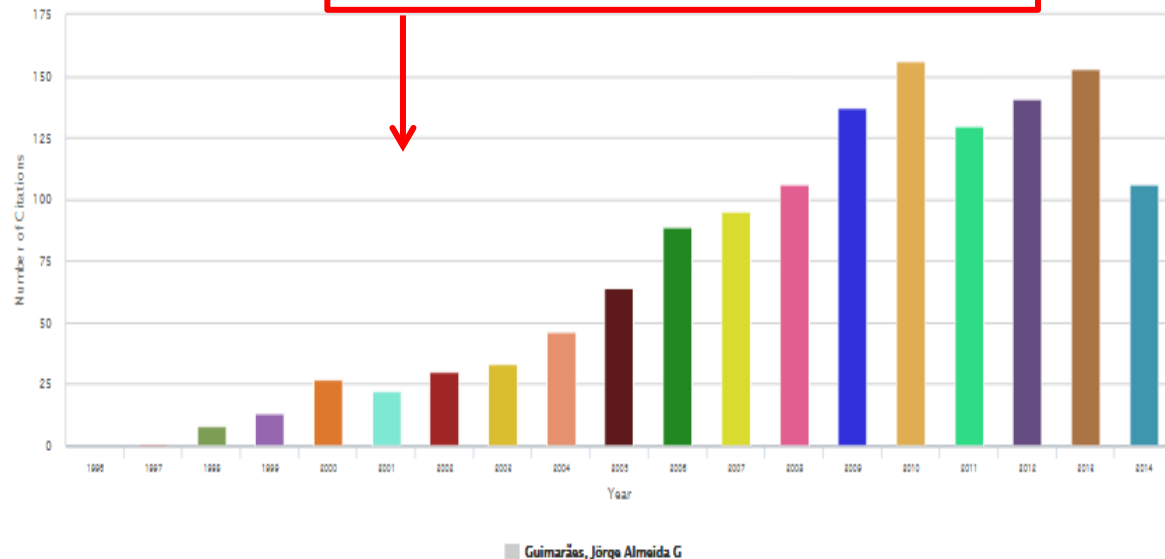
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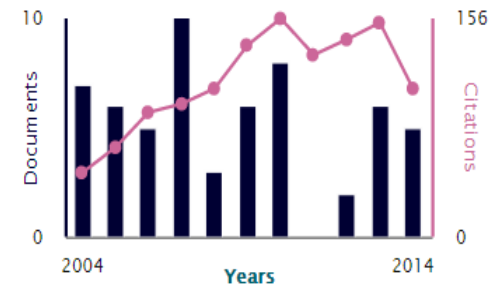
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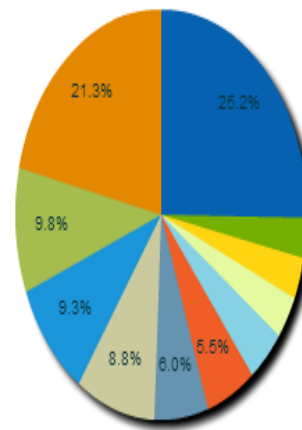
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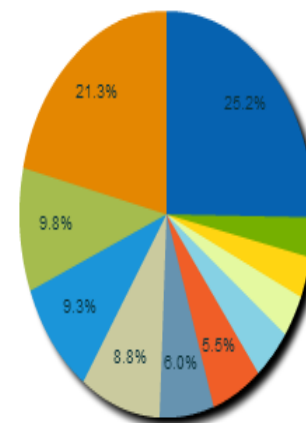
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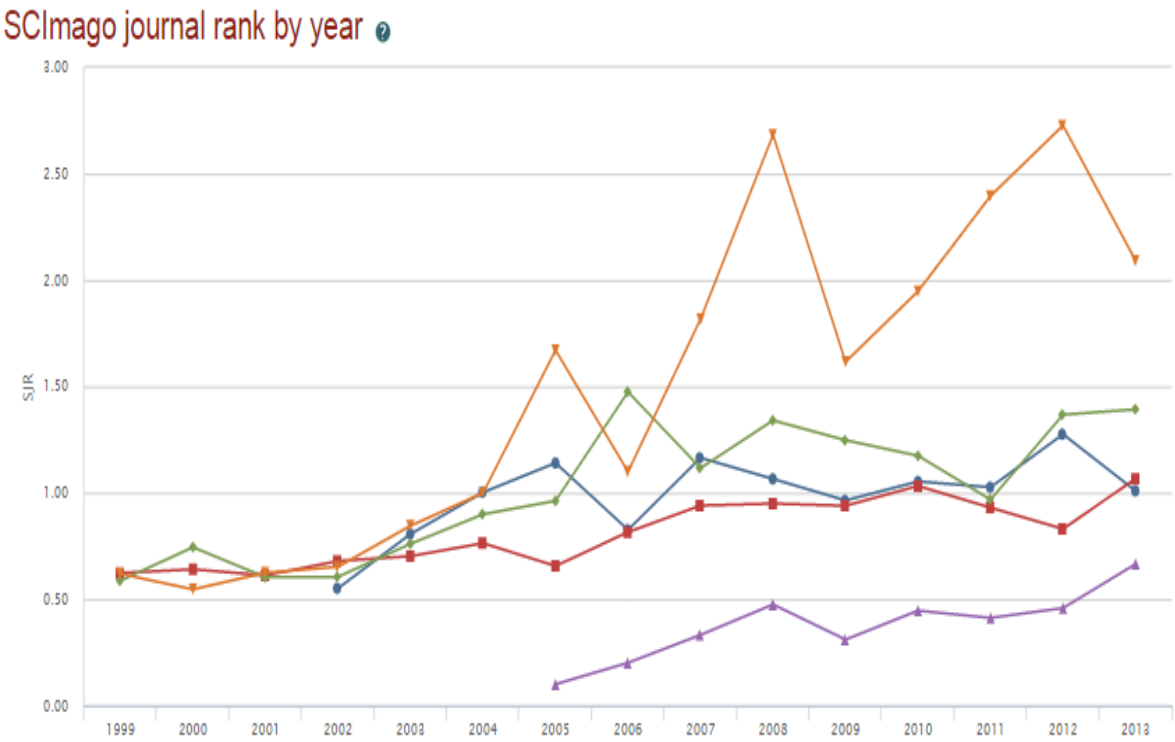
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