

SANTIAGO MELCHOR FERRER

Grupo de Investigación: **MODELIZACION Y DISEÑO MOLECULAR (Cod.: FQM174)**

Departamento: Universidad de Granada. Centro de Servicios de Informática y Redes de Comunicaciones

Código ORCID: <http://orcid.org/0000-0003-2499-3185>

RG: https://www.researchgate.net/profile/Santiago_Melchor

Correo electrónico: smelchor@ugr.es

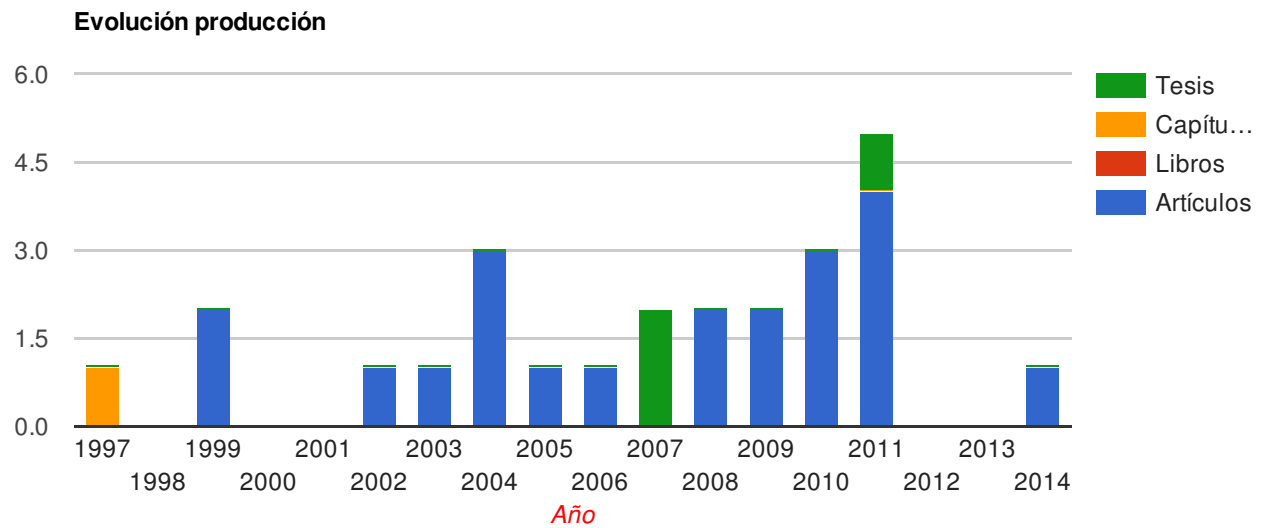
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Ficha del Directorio

Producción 25

Artículos (21) Libros (0) Capítulos de Libros (1) Tesis dirigidas (3)



Proyectos dirigidos 0

Proyectos (0) Contratos (0) Convenios (0)

Actividades 0

Titulo publicación	Fuente	Tipo	Fecha
Designing novel nanoporous architectures of carbon nanotubes for hydrogen storage	International journal of hydrogen energy	Articulo	2014
Contub v2.0 - algorithms for constructing c3-symmetric models of three-nanotube junctions	Journal of chemical information and modeling	Articulo	2011
Edge effects, electronic arrangement, and aromaticity patterns on finite-length carbon nanotubes	Physical chemistry chemical physics	Articulo	2011
Modelización molecular de nanotubos de carbono	Universidad de granada. química orgánica	Tesis doctoral	2011
N, p and as ylides and aza- and arsa-wittig reactions from topological analyses of electron density	The journal of physical chemistry part a: molecules, spectroscopy, kinetics, environment and general theory	Articulo	2011
Reversible attachment of platinum alloy nanoparticles to nonfunctionalized carbon nanotubes	Acs nano	Articulo	2011
Causes of energy destabilization in carbon nanotubes with topological defects	Theoretical chemistry accounts	Articulo	2010
Porous nanotube network: a novel 3-d nanostructured material with enhanced hydrogen storage capacity	Chemical communications	Articulo	2010
Reversible attachment of platinum alloy nanoparticles to nonfunctionalized carbon nanotubes	Acs nano	Articulo	2010
Crystal-growth behaviour in ca-mg-carbonate bacterial spherulites.	Crystal growth and design	Articulo	2009
Carbon...carbon weak interactions	The journal of physical chemistry part a: molecules, spectroscopy, kinetics, environment and general theory	Articulo	2009
Clar-kekule structuring in armchair carbon nanotubes	Organic letters	Articulo	2008
Evidence of an unexpectedly long c-c bond (> 2.7 angstrom) in 1,3-metalladiyne complexes [cp2mccr](2) (m = ti, zr): qtaim and elf analyses	The journal of physical chemistry part a: molecules, spectroscopy, kinetics, environment and general theory	Articulo	2008
Caracterización del enlace químico en compuestos de boro, iluros y reacciones de aza- y arsa-wittig: qtaim y análisis elf de la densidad electrónica.	Universidad de granada. química orgánica	Tesis doctoral	2007
Estudio computacional sobre la naturaleza del enlace carbono-metal	Universidad de granada. química orgánica	Tesis doctoral	2007
On the existence of alpha-agostic bonds: bonding analyses of titanium alkyl complexes	Organometallics	Articulo	2006
On the nature of metal-carbon bonding: aim and elf analyses of mchn (n=1-3) compounds containing early transition metals	The journal of physical chemistry part a: molecules, spectroscopy, kinetics, environment and general theory	Articulo	2005
Chemical bonding to n, p and as in ylides and their boron analogs	The journal of physical chemistry part a: molecules, spectroscopy, kinetics, environment and general theory	Articulo	2004
Contub: an algorithm for connecting two arbitrary carbon nanotubes	Journal of chemical information and computer sciences	Articulo	2004
Structure and theoretical nmr chemical shifts of modified cyclodextrins	Journal of molecular structure. theochem	Articulo	2004
Bonding of atomic phosphorus to polycyclic hydrocarbons and curved graphitic surfaces	Journal of physics and chemistry of solids	Articulo	2003
Structural and electronic effects of the interaction of metal cations with benzene	Journal of molecular structure. theochem	Articulo	2002
Geometry of multi-tube carbon clusters and electronic transmission in nanotube contacts	Molecular engineering	Articulo	1999
Theoretical calculations on c30h12 bowl-shaped			

hydrocarbons: nmr shielding constants, stability, and aromaticity	Journal of computational chemistry	Articulo	1999
Klasternye sistemy i materialy (sistemas y materiales cluster)	Isbn: 589238019x	Capítulo de libro	1997

	Titulo proyecto	Tipo	Inicio	Fin
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Actividades 0

Titulo actividad	Fuente	Tipo	Fecha
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Colaboradores

- JOSE ANTONIO DOBADO JIMENEZ (20)
- ISAAC VIDAL DAZA (4)
- AGUSTIN MARTIN ALGARRA (1)
- ANTONIO SÁNCHEZ NAVAS (1)
- JOSÉ DANIEL MARTÍN RAMOS (1)
- MARIA ANGUSTIAS RIVADENEIRA RUIZ (1)