



Nombres:

CARLOS ALBERTO

Apellidos:

CÁRDENAS VALENCIA

Título Profesional o Grado Académico (incluya el año de obtención):

INGENIERO MECÁNICO, 2003, COLOMBIA

Estudios de Postgrado o Especialización (institución donde lo obtuvo y año de obtención):

**DOCTOR EN CIENCIAS EXACTAS C/M QUÍMICA, 2007
UNIVERSIDAD ANDRÉS BELLO, CHILE - DOCTOR EN QUÍMICA, 2007,
UNIVERSIDAD ANDRÉS BELLO, CHILE**

Actividad Actual e Institución en la cual trabaja:

**PROFESOR INSTRUCTOR DEL DEPARTAMENTO DE FÍSICA DE LA
FACULTAD DE CIENCIAS**

Reseña de su actividad laboral actual:

Especialidad: Física Teórica

Temas de Investigación: Química Teórica

Docencia e investigación: atomic and molecular physics; theoretical chemical physics; theoretical chemistry; density function theory; ab initio electronic structure; theoretical and computational chemistry; theoretical and computational materials science

PUBLICACIONES:

Echegaray, E., Cárdenas, C., Rabi, S., Rabi, N., Lee, S., Zadeh, F.H., Toro-Labbe, A., Anderson, J.S.M., Ayers, P.W.

In pursuit of negative Fukui functions: Examples where the highest occupied molecular orbital fails to dominate the chemical reactivity

(2013) *Journal of Molecular Modeling*, 19 (7), pp. 2779-2783.

[http://www.scopus.com/inward/record.url?eid=2-s2.0-](http://www.scopus.com/inward/record.url?eid=2-s2.0-84879785879&partnerID=40&md5=a1525a146ce967a574c69f040527a518)

[84879785879&partnerID=40&md5=a1525a146ce967a574c69f040527a518](http://www.scopus.com/inward/record.url?eid=2-s2.0-84879785879&partnerID=40&md5=a1525a146ce967a574c69f040527a518)

DOCUMENT TYPE: Conference Paper

SOURCE: Scopus

Fuentealba, P., Cárdenas, C.

On the exponential model for energy with respect to number of electrons

(2013) *Journal of Molecular Modeling*, 19 (7), pp. 2849-2853.

[http://www.scopus.com/inward/record.url?eid=2-s2.0-](http://www.scopus.com/inward/record.url?eid=2-s2.0-84879788182&partnerID=40&md5=ee1a40d782ec47a9c609b9ca22dbec2c)

[84879788182&partnerID=40&md5=ee1a40d782ec47a9c609b9ca22dbec2c](http://www.scopus.com/inward/record.url?eid=2-s2.0-84879788182&partnerID=40&md5=ee1a40d782ec47a9c609b9ca22dbec2c)

DOCUMENT TYPE: Conference Paper

SOURCE: Scopus

Ayers, P.W., Cárdenas, C.

Communication: A case where the hard/soft acid/base principle holds regardless of acid/base strength

(2013) *Journal of Chemical Physics*, 138 (18), art. no. 181106, .

[http://www.scopus.com/inward/record.url?eid=2-s2.0-](http://www.scopus.com/inward/record.url?eid=2-s2.0-84877936394&partnerID=40&md5=0230c378f4c6e990b1ef6440a594b844)

[84877936394&partnerID=40&md5=0230c378f4c6e990b1ef6440a594b844](http://www.scopus.com/inward/record.url?eid=2-s2.0-84877936394&partnerID=40&md5=0230c378f4c6e990b1ef6440a594b844)

DOCUMENT TYPE: Article

SOURCE: Scopus

Muñoz, F., Cardenas, C., Rogan, J., Valdivia, J.A., Fuentealba, P., Kiwi, M.

Ab initio molecular dynamics simulations of Ti₂ on C₂₀ collisions and C₂₀Ti₂ configurations

(2013) *Journal of Physical Chemistry C*, 117 (8), pp. 4287-4291.

[http://www.scopus.com/inward/record.url?eid=2-s2.0-](http://www.scopus.com/inward/record.url?eid=2-s2.0-84874603694&partnerID=40&md5=a0df8391452ab6b70606fc4ed15876bc)

[84874603694&partnerID=40&md5=a0df8391452ab6b70606fc4ed15876bc](http://www.scopus.com/inward/record.url?eid=2-s2.0-84874603694&partnerID=40&md5=a0df8391452ab6b70606fc4ed15876bc)

DOCUMENT TYPE: Article

SOURCE: Scopus

Cárdenas, C., Muñoz, F., Muñoz, M., Bernardin, A., Fuentealba, P.

A new isomer of C₂₀ and a way to a new C₂₄₀

(2012) *Physical Chemistry Chemical Physics*, 14 (43), pp. 14810-14814. Cited 1 time.

[http://www.scopus.com/inward/record.url?eid=2-s2.0-](http://www.scopus.com/inward/record.url?eid=2-s2.0-84867700071&partnerID=40&md5=4856ffb0fba35afac4e0c327961476f4)

[84867700071&partnerID=40&md5=4856ffb0fba35afac4e0c327961476f4](http://www.scopus.com/inward/record.url?eid=2-s2.0-84867700071&partnerID=40&md5=4856ffb0fba35afac4e0c327961476f4)

DOCUMENT TYPE: Article

SOURCE: Scopus

Cuevas-Saavedra, R., Chakraborty, D., Rabi, S., Cárdenas, C., Ayers, P.W.

Symmetric nonlocal weighted density approximations from the exchange-correlation hole of the uniform electron gas

(2012) *Journal of Chemical Theory and Computation*, 8 (11), pp. 4081-4093. Cited 2 times.

[http://www.scopus.com/inward/record.url?eid=2-s2.0-](http://www.scopus.com/inward/record.url?eid=2-s2.0-84869068776&partnerID=40&md5=3b9e59fd0ddc97319632e43c83d5c7bb)

[84869068776&partnerID=40&md5=3b9e59fd0ddc97319632e43c83d5c7bb](http://www.scopus.com/inward/record.url?eid=2-s2.0-84869068776&partnerID=40&md5=3b9e59fd0ddc97319632e43c83d5c7bb)

DOCUMENT TYPE: Article

SOURCE: Scopus

Chakraborty, D., Cárdenas, C., Echegaray, E., Toro-Labbe, A., Ayers, P.W.

Understanding chemical binding using the Berlin function and the reaction force

(2012) *Chemical Physics Letters*, 539-540, pp. 168-171. Cited 2 times.

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84862653228&partnerID=40&md5=dd84dddef3e72c2721c364890f350143>
DOCUMENT TYPE: Article
SOURCE: Scopus

Osorio, E., Ferraro, M.B., Oña, O.B., Cardenas, C., Fuentealba, P., Tiznado, W.
Assembling small silicon clusters using criteria of maximum matching of the Fukui functions
(2011) *Journal of Chemical Theory and Computation*, 7 (12), pp. 3995-4001.
<http://www.scopus.com/inward/record.url?eid=2-s2.0-83455224952&partnerID=40&md5=baa0a310b85065bddf7a4382272e9e8a>
DOCUMENT TYPE: Article
SOURCE: Scopus

Cárdenas, C.
The Fukui potential is a measure of the chemical hardness
(2011) *Chemical Physics Letters*, 513 (1-3), pp. 127-129. Cited 1 time.
<http://www.scopus.com/inward/record.url?eid=2-s2.0-80052272046&partnerID=40&md5=d5563ed9b96594556075b9843a0e21bc>
DOCUMENT TYPE: Article
SOURCE: Scopus

Cárdenas, C., Tiznado, W., Ayers, P.W., Fuentealba, P.
The Fukui potential and the capacity of charge and the global hardness of atoms
(2011) *Journal of Physical Chemistry A*, 115 (11), pp. 2325-2331. Cited 7 times.
<http://www.scopus.com/inward/record.url?eid=2-s2.0-79952743956&partnerID=40&md5=4baf50973797014a8f5ac75e01ea5907>
DOCUMENT TYPE: Article
SOURCE: Scopus

Cárdenas, C., Ayers, P., De Proft, F., Tozer, D.J., Geerlings, P.
Should negative electron affinities be used for evaluating the chemical hardness?
(2011) *Physical Chemistry Chemical Physics*, 13 (6), pp. 2285-2293. Cited 12 times.
<http://www.scopus.com/inward/record.url?eid=2-s2.0-79251570907&partnerID=40&md5=c99e66b838f175cc4fd2b425a7611413>
DOCUMENT TYPE: Article
SOURCE: Scopus

Cárdenas, C., Rabi, N., Ayers, P.W., Morell, C., Jaramillo, P., Fuentealba, P.
Chemical reactivity descriptors for ambiphilic reagents: Dual descriptor, local hypersoftness, and electrostatic potential
(2009) *Journal of Physical Chemistry A*, 113 (30), pp. 8660-8667. Cited 28 times.
<http://www.scopus.com/inward/record.url?eid=2-s2.0-67651148133&partnerID=40&md5=165c09f2d15507575254398b01cd9a18>
DOCUMENT TYPE: Article
SOURCE: Scopus

Cárdenas, C., Echegaray, E., Chakraborty, D., Anderson, J.S.M., Ayers, P.W.
Relationships between the third-order reactivity indicators in chemical density-functional theory
(2009) *Journal of Chemical Physics*, 130 (24), art. no. 244105, . Cited 7 times.
<http://www.scopus.com/inward/record.url?eid=2-s2.0-67650459102&partnerID=40&md5=3d0e90ba0bc301e76336813423da9768>
DOCUMENT TYPE: Article
SOURCE: Scopus

Cárdenas, C., De Proft, F., Chamorro, E., Fuentealba, P., Geerlings, P.
Theoretical study of the surface reactivity of alkaline earth oxides: Local density of states evaluation of the local softness
(2008) *Journal of Chemical Physics*, 128 (3), art. no. 034708, . Cited 9 times.
<http://www.scopus.com/inward/record.url?eid=2-s2.0-38349144301&partnerID=40&md5=f8847ddcc1593b5b7c3a7cf532a97a12>
DOCUMENT TYPE: Article
SOURCE: Scopus

Alzate-Morales, J.H., Tiznado, W., Santos, J.C., Cárdenas, C., Contreras, R.
Theoretical study on CDK2 inhibitors using a global softness obtained from the density of states
(2007) *Journal of Physical Chemistry B*, 111 (12), pp. 3293-3297. Cited 4 times.
<http://www.scopus.com/inward/record.url?eid=2-s2.0-34147110853&partnerID=40&md5=dd8ea7a672f1eabe8e99396765ffa239>
DOCUMENT TYPE: Article
SOURCE: Scopus

Fuentealba, P., Chamorro, E., Cárdenas, C.
Further exploration of the Fukui function, hardness, and other reactivity indices and its relationships within the Kohn-Sham scheme
(2007) *International Journal of Quantum Chemistry*, 107 (1), pp. 37-45. Cited 16 times.
<http://www.scopus.com/inward/record.url?eid=2-s2.0-33751539853&partnerID=40&md5=aabf30129681b1f89d9050b430295ccc>
DOCUMENT TYPE: Article
SOURCE: Scopus

Cárdenas, C., Lamsabhi, A.M., Fuentealba, P.
Nuclear reactivity indices in the context of spin polarized density functional theory
(2006) *Chemical Physics*, 322 (3), pp. 303-310. Cited 9 times.
<http://www.scopus.com/inward/record.url?eid=2-s2.0-33644755676&partnerID=40&md5=bd9ab11112bf3862d089665671b9048a>
DOCUMENT TYPE: Article
SOURCE: Scopus

Chamorro, E., Duque, M., Cárdenas, C., Santos, J., Tiznado, W., Fuentealba, P.
Condensation of the highest occupied molecular orbital within the electron localization function domains
(2005) *Journal of Chemical Sciences*, 117 (5), pp. 419-424. Cited 3 times.
<http://www.scopus.com/inward/record.url?eid=2-s2.0-27844531583&partnerID=40&md5=e74e215e09f6b06e40a86c13ec710cab>
DOCUMENT TYPE: Article
SOURCE: Scopus

Cárdenas, C., Chamorro, E., Notario, R.
Nature of bonding in the cyclization reactions of (2-Ethynylphenyl)triazene and 2-ethynylstyrene
(2005) *Journal of Physical Chemistry A*, 109 (19), pp. 4352-4358. Cited 20 times.
<http://www.scopus.com/inward/record.url?eid=2-s2.0-19944363191&partnerID=40&md5=78751f103d80c8efdc4c94c2533300c9>
DOCUMENT TYPE: Article
SOURCE: Scopus

PROYECTOS DE INVESTIGACIÓN:

- COINVESTIGADOR, EXPLORING THE DYNAMICS AND REACTIVITY OF ATOMIC AND MOLECULAR CLUSTERS. FONDECYT 1130202, 2013
- INVESTIGADOR RESPONSIBLE, DESCRIBING THE REACTIVITY OF COMPLEX MOLECULAR SYSTEMS. FONDECYT 11090013, 2009

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