

## Curriculum vitae

### Personal data:

- full name: Lucian Aurel Constantin
- data & place of birth : ~~October 29, 1949, Bucharest, Romania~~
- languages: Romanian (native), English, French, Italian
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- Identifiers :
  - Web of Science ResearcherID **E-6271-2012**
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  - <https://scholar.google.com/citations?user=aQ4cCtEAAAJ&hl=it>

### Academic education :

- 1988 - 1993 : Bachelor's degree in physics, Bucharest University, Romania, advisor : Prof. Ciobanu Constantin
- 1998 - 2000 : M. Sc. in physics, University of Puerto Rico, Rio Piedras, San Juan, Puerto Rico
  - CUM GPA: 4. (100 %)
  - research in General Relativity Theory, advisor: Prof. Ponce de Leon
  - Thesis: *Induced matter from a 5-dimensional Kaluza-Klein theory*
- 2000-2006 : PhD in Physics, Tulane University, New Orleans, USA
  - CUM GPA : 3.867 (96.675 %)
  - PhD Preliminary exam (passed with distinction)
  - research in Density Functional Theory, advisor Prof. John P. Perdew
  - Thesis : *Meta-generalized exchange-correlation hole model and a Laplacian-level kinetic energy functional*

### Last position :

- work place : Italian Institute of Technology (IIT), Via Barsanti, I-73010 Arnesano, Italy
- work position : April 2010 – April 2020: team leader and researcher, Italian Institute of Technology, Center for biomolecular nanotechnology, Research in Density Functional Theory, with applications in Quantum Chemistry and Solid-State Physics, in the group of Prof. Fabio Della Sala ;

### Previous research experience :

- 2003-2005 : research in Numerical Methods for Time-Dependent PDE's, Hyperbolic Systems of Conservation Laws; advisor Prof. Alexander Kurganov, Tulane University, Mathematics Department
- 2000-2002 : research in Biophysics : Ion Channels, advisor Prof. Mark Millonas and Prof. Armin Kargol, Tulane University, Physics Department
- 2006-2007 : pos-doc, Donostia International Physics Center (DIPC), Basque Country, Spain, Research in High-level-orbital-dependent-methods applied in Surface Science, advisor J.M. Pitarke ;
- 2007-2009 : pos-doc, Tulane University, New Orleans, USA, Physics Department, Research in Density Functional Theory- Fundamentals, advisor Prof. John Perdew ;
- 2009-2010 : pos-doc, University of California at Irvine (UCI), USA, Chemistry Department, Research in Density Functional Theory – Fundamentals, advisor Prof. Kieron Burke ;

## Academic and teaching experience :

2005-2006 : Research Assistant, Tulane University, Physics Department (and, September 12- December 19, visiting student at Rice University, Chemistry Department, in the theoretical group of Prof. Gustavo Scuseria)

2000 – 2005 : Teaching Assistant, Tulane University, Physics Department

1998 – 2000 : Teaching Assistant, University of Puerto Rico, Physics Department

1994 – 1998 : Physics Professor, high school, Bucharest, Romania

## Internationally established conferences and workshops:

### (Poster and talk sessions) :

**Contributed Talk :** *Van der Waals functional for bulk solids*, 17th International Conference on Density-Functional Theory and its Applications (21- 25 August 2017, Sweden).

**Invited Talk :** *Semiclassical atom theory applied to solid-state physics*, 2017 Sanibel Symposium, February 19-24, St. Simons Island, USA.

**Invited Talk :** *Semilocal density functional theory with correct surface asymptotics*, 2016 EMN Meeting on Computation and Theory, October 10-14 Las Vegas, USA.

**Poster :** *New exact conditions for density functionals*, Psi-K Conference 2015, September 6-10, San Sebastian, Spain.

**Poster :** *Global hybrids from the semiclassical atom theory satisfying the local density linear response*, Psi-K Conference 2015, September 6-10, San Sebastian, Spain.

**Invited Talk :** *Novel exchange-correlation density functionals and their utility in nano-science*, 2015 EMN/Spain Meeting, September 1-4 San Sebastian, Spain.

**Contributed Talk :** *Improving atomization energies of molecules and solids with a spin-dependent gradient correction from one-electron density analysis*, CECAM workshop : Spin states in biochemistry and inorganic chemistry, 18-21 September 2012, Zaragoza, Spain.

**Contributed Talk :** *Semiclassical Neutral Atom as a Reference System in Density Functional Theory*, Symposium *Challenges in Density Matrix and Density Functional Theory* , 1-6 April 2012, Ghent, Belgium.

**Poster :** *Semiclassical Neutral Atom as a Reference System in Density Functional Theory*, CECAM DFT workshop : How to Speed Up Progress and Reduce Empiricism, 2011.

**Poster :** *Exchange-correlation energy functional based on the Airy-gas reference system*, Psi-k Conference, 2010.

**Poster :** *Ionization potentials in the limit of large atomic number*, KITP Conference: From Basic Concepts to Real Materials, 2009.

**Poster :** *Dimensional crossover of the exchange-correlation energy at the semilocal level*, Gordon Research Conference, Time-Dependent Density Functional Theory, 2009.

**Contributed Talk :** *High-Level Correlated Approach to the Jellium Surface Energy, without Uniform-Gas Input* , March APS Meeting, 2008.

**Poster :** *Kinetic energy density functionals from the Airy gas with an application to the atomization kinetic energies of molecules*, March APS Meeting, 2008.

**Poster :** *Meta-generalized gradient approximation for the exchange-correlation hole with an application to the jellium surface energy*, at Fifth Congress of the International Society for Theoretical Chemical Physics, 2005.

## Invited work and seminar sessions :

- one week in the group of Prof. J.M. Pitarke, Donostia International Physics Center (DIPC), work done for *Adiabatic-connection-fluctuation-dissipation approach to long-range behavior of exchange-correlation energy at metal surfaces: A numerical study for jellium slabs*, 2010.
- one week in the group of Prof. Kieron Burke, University of California at Irvine (UCI), USA, Chemistry Department, work done for *Ionization potentials in the limit of large atomic number*, 2008. Seminar presentation : *Airy gas model in DFT development*
- two months in the group of Prof. Gustavo Scuseria, Rice University, Houston, USA, Chemistry

Department, work done for my PhD thesis, 2005. Seminar presentation : *Meta-GGA exchange-correlation hole model*

- invitation for Prof. Andreas Savin at the Italian Institute of Technology, in Lecce, work about short-range, long-range correlation energy of the gapped uniform electron gas, 2014.
- one week in the group of Prof. J.M. Pitarke, Donostia International Physics Center (DIPC), establishing a collaboration for construction of exchange-correlation kernels, 2015.

**Society Membership:** American Physical Society

### **Academic Service :**

**Reviewer for:** Physical Review Letters, Physical Review B, The Journal of Chemical Physics, Physica Scripta, Journal of Physics: Condensed Matter, Journal of Physics B: Atomic, Molecular & Optical Physics, Journal of Computational Chemistry, Crystal Growth & Design, Journal of Chemical Theory and Computation

### **Research Record Statistics (using Web of Science and Google Scholar) :**

- **published articles : 73**

PHYSICAL REVIEW B	30
PHYSICAL REVIEW LETTERS	11
THE JOURNAL OF PHYSICAL CHEMISTRY LETTERS	1
JOURNAL OF CHEMICAL THEORY AND COMPUTATION	11
JOURNAL OF CHEMICAL PHYSICS	7
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY	2
THEORETICAL CHEMISTRY ACCOUNTS	1
PROGRESS IN THEORETICAL CHEMISTRY AND PHYSICS	1
PHYSICAL REVIEW A	2
JOURNAL OF PHYSICS : CONDENSED MATTER	1
GENERAL PHYSIOLOGY AND BIOPHYSICS	1
COMPUTATION	3
ADVANCES IN THE THEORY OF ATOMIC AND MOLECULAR SYSTEMS	
CONCEPTUAL AND COMPUTATIONAL ADVANCES IN QUANTUM CHEMISTRY	1
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY	1

- **Sum of the times cited :** Web of Science : 6299; Google Scholar : 7919
- **h-index :** Web of Science : 28 ; Google Scholar : 30
- **i10-index :** Google Scholar : 54

## Research Activity :

I have large expertise in the development of ground-state Density Functional Theory (DFT) and high-level, orbital-dependent methods in context of linear-response time-dependent DFT approach, having the opportunity to work with Prof. John Perdew (one of DFT pioneers), that has been my PhD supervisor at Tulane University ; with Prof. Kieron Burke, Prof. J.M. Pitarke, and Prof. Fabio Della Sala. In the last five years, I strongly collaborated also with the team member Dr. Eduardo Fabiano, which is an expert of DFT and computational quantum chemistry. I have published important work in electronic structure calculations, and I am co-author of the following functionals :

- exchange-correlation generalized gradient approximations (GGAs) : PBEsol ([8]), zPBEsol ([30]), PBEint ([20]), APBE ([27]), q2D ([29]), SG4 ([45])
- exchange-correlation meta-GGAs : revTPSS ([19]), BLOC ([35])
- exchange-correlation hybrids : hPBEint ([31]), hAPBE ([40])
- exchange-correlation kernels for time-dependent DFT : CP ([4]), JGM ([33]), NEO ([50]), q2D[46]
- kinetic energy functionals for the subsystem DFT: GGAs (e.g. [25], [53]), and Laplacian-meta-GGAs ([36], [43], [52])
- kinetic energy functionals for orbital-free DFT (e.g. [5])
- we have also proposed a new kind of functional, denoted u-meta-GGA, that depends on the meta-GGA ingredients, as well as the reduced Hartree potential. The exchange u-meta-GGA functional [49] is always exact for any one- and two-electron systems, while the kinetic u-meta-GGA functional [54] shows an improved performance with respect to GGA and meta-GGA functionals.

All these functionals have been constructed from exact quantum mechanics conditions, without (or with minimal) empiricism. I have studied quantum mechanics exact conditions and model systems, such as :

- density scalings ([32])
- semiclassical physics ([3], [45])
- uniform electron gas with gap model ([33], [37], [53])
- Airy gas model ([11], [13], [14])
- jellium surfaces ([1], [2], [7], [15], [22], [23], [50])
- asymptotic and nuclear properties of the kinetic and exchange energies ([41], [47])
- quasi-two-dimensional conditions for exchange and correlation ([6], [9], [29], [46])
- gradient-dependent upper bound of the exchange-correlation energy ([42])

I have also contributed to several real applications studies:

- we proposed a benchmark data for dihydrogen complexes ([39]), we constructed our own benchmark set, with a large number of molecular systems and many energetic and geometrical ground-state properties, used for testing our functionals (e.g. [35], [40])
- we studied various interesting systems (e.g. gold nanostructures ([24])



## List of Most Relevant Published Articles (chronological order):

[69] S Jana, A Patra, LA Constantin, P Samal, *Screened range-separated hybrid by balancing the compact and slowly varying density regimes: Satisfaction of local density linear response*, **The Journal of Chemical Physics** 152 (4), 044111 (2020).

[68] S Jana, LA Constantin, P Samal, *Accurate water properties from an efficient ab-initio method*, **Journal of Chemical Theory and Computation** (2020).

[67] AV Terentjev, LA Constantin, E Artacho, JM Pitarke, *Comparison of dispersion-corrected exchange-correlation functionals using atomic orbitals*, **Physical Review B** 100 (23), 235439 (2019).

[66] S Śmiga, LA Constantin, F Della Sala, E Fabiano, *The Role of the Reduced Laplacian Renormalization in the Kinetic Energy Functional Development*, **Computation** 7 (4), 65 (2019).

[65] B Patra, S Jana, LA Constantin, P Samal, *Relevance of the Pauli kinetic energy density for semilocal functionals*, **Physical Review B** 100 (15), 155140 (2019).

[64] B Patra, S Jana, LA Constantin, P Samal, *Efficient band gap prediction of semiconductors and insulators from a semilocal exchange-correlation functional*, **Physical Review B** 100 (4), 045147 (2019).

[63] S Jana, A Patra, LA Constantin, H Myneni, P Samal, *Long-range screened hybrid-functional theory satisfying the local-density linear response*, **Physical Review A** 99 (4), 042515 (2019).

[62] LA Constantin, *Semilocal properties of the Pauli kinetic potential*, **Physical Review B** 99 (15), 155137 (2019).

[61] LA Constantin, E Fabiano, F Della Sala, *Performance of semilocal kinetic energy functionals for Orbital-Free Density Functional Theory*, **Journal of chemical theory and computation** 15 (5), 3044-3055 (2019).

[60] LA Constantin, *Correlation energy functionals from adiabatic connection formalism*, **Physical Review B** 99 (8), 085117 (2019).

[59] AV Terentjev, LA Constantin, JM Pitarke, *Dispersion-corrected PBEsol exchange-correlation functional*, **Physical Review B** 98 (21), 214108 (2018).

[58] AV Terentjev, LA Constantin, JM Pitarke, *Gradient-dependent exchange-correlation kernel for materials optical properties*, **Physical Review B** 98 (8), 085123 (2018).

[57] LA Constantin, E Fabiano, F Della Sala, *Semilocal Pauli-Gaussian kinetic functionals for orbital-free density functional theory calculations of solids*, **The journal of physical chemistry letters** 9 (15), 4385-4390 (2018).

[56] LA Constantin, E Fabiano, F Della Sala, *Nonlocal kinetic energy functional from the jellium-with-gap model: Applications to orbital-free density functional theory*,

**Physical Review B 97 (20), 205137 (2018).**

[55] AV Terentjev, P Cortona, LA Constantin, JM Pitarke, F Della Sala, E. Fabiano, *Solid-state testing of a van-der-waals-corrected exchange-correlation functional based on the semiclassical atom theory*, **Computation 6 (1), 7 (2018).**

[54] Lucian A. Constantin, Eduardo Fabiano, and Fabio Della Sala, *Modified fourth-order kinetic energy gradient expansion with Hartree potential dependent coefficients*, **J. Chem. Theory Comput. 13 (9), 4228-4239 (2017).**

[53] Lucian A. Constantin, Eduardo Fabiano, Szymon Śmiga, and Fabio Della Sala, *Jellium-with-gap model applied to semilocal kinetic functionals*, **Phys. Rev. B 95, 115153 (2017).**

[52] Szymon Śmiga, Eduardo Fabiano, Lucian A. Constantin, and Fabio Della Sala, *Laplacian-dependent models of the kinetic energy density: Applications in subsystem density functional theory with meta-generalized gradient approximation functionals*, **J. Chem. Phys. 146, 064105 (2017).**

[51] Fabio Della Sala, Eduardo Fabiano, and Lucian A. Constantin, *Review: Kinetic-energy-density dependent semilocal exchange-correlation functionals*, **Int. J. Quantum Chem. 116, 1641 (2016).**

[50] Adrienn Ruzsinszky, Lucian A. Constantin, and J. M. Pitarke, *Kernel-corrected random-phase approximation for the uniform electron gas and jellium surface energy*, **Phys. Rev. B 94, 165155 (2016).**

[49] Lucian A. Constantin, Eduardo Fabiano, and Fabio Della Sala, *Hartree potential dependent exchange functional*, **J. Chem. Phys. 145, 084110 (2016).**

[48] Lucian A. Constantin, Eduardo Fabiano, and Fabio Della Sala, *Kinetic and Exchange Energy Densities near the Nucleus*, **Computation 4, 19 (2016).**

[47] Lucian A. Constantin, Eduardo Fabiano, J. M. Pitarke, and Fabio Della Sala, *Semilocal density functional theory with correct surface asymptotics*, **Phys. Rev. B 93, 115127 (2016).**

[46] Lucian A. Constantin, *Simple effective interaction for dimensional crossover*, **Phys. Rev. B 93, 121104(R) (2016).**

[45] Lucian A. Constantin, Aleksandrs Terentjevs, Fabio Della Sala, Pietro Cortona, and Eduardo Fabiano, *Semiclassical atom theory applied to solid-state physics*, **Phys. Rev. B 93, 045126 (2016).**

[44] E. Fabiano, L.A. Constantin, A. Terentjevs, F. Della Sala, and P. Cortona, *Assessment of the TCA functional in computational chemistry and solid-state physics*, **Theor. Chem. Acc. 134 (2015).**

[43] Szymon Śmiga, Eduardo Fabiano, Savio Laricchia, Lucian A. Constantin, and Fabio Della Sala, *Subsystem density functional theory with meta-generalized gradient approximation exchange-correlation functionals*, **J. Chem. Phys. 142, 154121 (2015).**

[42] Lucian A. Constantin, Aleksandrs Terentjevs, Fabio Della Sala, and Eduardo Fabiano, *Gradient-dependent upper bound for the exchange-correlation energy and application to density functional theory*, **Phys. Rev. B. 91, 041120 (R) (2015).**

[41] Fabio Della Sala, Eduardo Fabiano, and Lucian A. Constantin, *Kohn-Sham kinetic energy density in the nuclear and asymptotic regions: Deviations from the von Weizsacker behavior and application to density functionals*, **Phys. Rev. B 91, 035126 (2015).**

- [40] Eduardo Fabiano, Lucian A. Constantin, Pietro Cortona, and Fabio Della Sala, *Global hybrids from the semiclassical atom theory satisfying the local density linear response*, **J. Chem. Theory Comput.** **11**, 122 (2015).
- [39] Eduardo Fabiano, Lucian A. Constantin, and Fabio Della Sala, *Wave Function and Density Functional Theory studies of Dihydrogen Complexes*, **J. Chem. Theory Comput.** **10**, 3151, 2014.
- [38] Aleksandrs Terentjevs, Paolo E. Trevisanutto, Lucian A. Constantin, and Fabio Della Sala, *First principles optical spectra of the beta-SiC(001)/Al interface*, **J. Phys. Condens. Matter** **26**, 265006, 2014.
- [37] Eduardo Fabiano, Aleksandrs Terentjevs, Paolo E. Trevisanutto, and Lucian A. Constantin, *Generalized Gradient Approximation Correlation Energy Functionals Based on the Uniform Electron Gas with Gap Model*, **J. Chem. Theory Comput.** **10**, 2016, 2014.
- [36] Savio Laricchia, Lucian A. Constantin, Eduardo Fabiano, and Fabio Della Sala, *Laplacian-Level Kinetic Energy Approximations Based on the Fourth-Order Gradient Expansion: Global Assessment and Application to the Subsystem Formulation of Density Functional Theory*, **J. Chem. Theory Comput.** **10**, 164, 2014.
- [35] Lucian A. Constantin, Eduardo Fabiano, and Fabio Della Sala, *Meta-GGA Exchange-Correlation Functional with a Balanced Treatment of Nonlocality*, **J. Chem. Theory Comput.** **9**, 2256, 2013.
- [34] Lucian A. Constantin, Eduardo Fabiano, and Fabio Della Sala, *Construction of a general semilocal exchange-correlation hole model: Application to nonempirical meta-GGA functionals*, **Phys. Rev. B** **88**, 125112, 2013.
- [33] Paolo E. Trevisanutto, Aleksandrs Terentjevs, Lucian A. Constantin, Valerio Olevano, and Fabio Della Sala, *Optical spectra of solids obtained by time-dependent density functional theory with the jellium-with-gap-model exchange-correlation kernel*, **Phys. Rev. B** **87**, 205143, 2013.
- [32] Eduardo Fabiano and Lucian A. Constantin, *Relevance of coordinate and particle-number scaling in density-functional theory*, **Phys. Rev. A** **87**, 012511, 2013.
- [31] Eduardo Fabiano, Lucian A. Constantin, and Fabio Della Sala, *Testing the broad applicability of the PBEint GGA functional and its one-parameter hybrid form*, **Int. J. Quantum Chem.** **113**, 673, 2013.
- [30] Lucian A. Constantin, Eduardo Fabiano, and Fabio Della Sala, *Spin-dependent gradient correction for more accurate atomization energies of molecules*, **J. Chem. Phys.** **137**, 194105, 2012.
- [29] Letizia Chiodo, Lucian A. Constantin, Eduardo Fabiano, and Fabio Della Sala, *Nonuniform Scaling Applied to Surface Energies of Transition Metals*, **Phys. Rev. Lett.** **108**, 126402, 2012.
- [28] Lucian A. Constantin, Eduardo Fabiano, and Fabio Della Sala, *Semilocal dynamical correlation with increased localization*, **Phys. Rev. B** **86**, 035130, 2012.
- [27] Lucian A. Constantin, E. Fabiano, S. Laricchia, and F. Della Sala, *Semiclassical Neutral Atom as a Reference System in Density Functional Theory*, **Phys. Rev. Lett.** **106**, 186406, 2011.
- [26] E. Fabiano, Lucian A. Constantin, and F. Della Sala, *Two-Dimensional Scan of the Performance of Generalized Gradient Approximations with Perdew–Burke–Ernzerhof-Like Enhancement Factor*, **J. Chem. Theory Comput.** **7**, 3548, 2011.
- [25] S. Laricchia, E. Fabiano, Lucian A. Constantin, and F. Della Sala, *Generalized Gradient Approximations of the Noninteracting Kinetic Energy from the Semiclassical Atom Theory: Rationalization of the Accuracy of the Frozen Density Embedding Theory for Nonbonded Interactions*, **J. Chem. Theory Comput.** **5**, 2439, 2011.

[24] E. Fabiano, Lucian A. Constantin, and F. Della Sala, *Exchange-correlation generalized gradient approximation for gold nanostructures*, **J. Chem. Phys.** **134**, 194112, 2011.

[23] Lucian A. Constantin, Letizia Chiodo, Eduardo Fabiano, Igor Bodrenko, and Fabio Della Sala *Correlation energy functional from jellium surface analysis*, **Phys. Rev. B** **84**, 045126, 2011.

[22] Lucian A. Constantin and J. M. Pitarke, *Adiabatic-connection-fluctuation-dissipation approach to long-range behavior of exchange-correlation energy at metal surfaces: A numerical study for jellium slabs* **Phys. Rev. B** **83**, 2011.

[21] Lucian A. Constantin, John C. Snyder, John P. Perdew, and Kieron Burke, *Communication: Ionization potentials in the limit of large atomic number*, **J. Chem. Phys.** **133**, 241103, 2010.

[20] Eduardo Fabiano, Lucian A. Constantin, and Fabio Della Sala, *Generalized gradient approximation bridging the rapidly and slowly varying density regimes: A PBE-like functional for hybrid interfaces*, **Phys. Rev. B** **82**, 113104, 2010.

[19] John P. Perdew, Adrienn Ruzsinszky, Gábor I. Csonka, Lucian A. Constantin, and Jianwei Sun, *Workhorse Semilocal Density Functional for Condensed Matter Physics and Quantum Chemistry*, **Phys. Rev. Lett.** **103**, 026403, 2009; (E) **Phys. Rev. Lett.** **106**, 179902, 2011.

[18] Lucian A. Constantin and J. M. Pitarke, *The Many-Body Exchange-Correlation Hole at Metal Surfaces*, **J. Chem. Theory Comput.** **5**, 895, 2009.

[17] John P. Perdew, Adrienn Ruzsinszky, Lucian A. Constantin, Jianwei Sun and Gábor I. Csonka, *Some Fundamental Issues in Ground-State Density Functional Theory: A Guide for the Perplexed*, **J. Chem. Theory Comput.** **5**, 902, 2009.

[16] Donghyung Lee, Lucian A. Constantin, John P. Perdew, and Kieron Burke, *Condition on the Kohn-Sham kinetic energy and modern parametrization of the Thomas-Fermi density*, **J. Chem. Phys.** **130**, 034107, 2009.

[15] C. M. Horowitz, Lucian A. Constantin, C. R. Proetto, and J. M. Pitarke, *Position-dependent exact-exchange energy for slabs and semi-infinite jellium*, **Phys. Rev. B** **80**, 235101, 2009.

[14] Lucian A. Constantin, Adrienn Ruzsinszky, and John P. Perdew, *Exchange-correlation energy functional based on the Airy-gas reference system*, **Phys. Rev. B** **80**, 035125, 2009.

[13] Lucian A. Constantin and Adrienn Ruzsinszky, *Kinetic energy density functionals from the Airy gas with an application to the atomization kinetic energies of molecules*, **Phys. Rev. B** **79**, 115117, 2009.

[12] Lucian A. Constantin, John P. Perdew, and J. M. Pitarke, *Exchange-correlation hole of a generalized gradient approximation for solids and surfaces*, **Phys. Rev. B** **79**, 075126, 2009.

[11] John P. Perdew, Lucian A. Constantin, Adrienn Ruzsinszky, *Energy Densities of Exchange and Correlation in the Slowly Varying Region of the Airy Gas*, **ADVANCES IN THE THEORY OF ATOMIC AND MOLECULAR SYSTEMS: CONCEPTUAL AND COMPUTATIONAL ADVANCES IN QUANTUM CHEMISTRY**, Book Series: **Progress in Theoretical Chemistry and Physics**, Volume: **19**, Pages: 297-310, 2009.

[10] John P. Perdew, Adrienn Ruzsinszky, Gábor I. Csonka, Oleg A. Vydrov, Gustavo E. Scuseria, Lucian A. Constantin, Xiaolan Zhou, and Kieron Burke, *Perdew et. al. Reply*, **Phys. Rev. Lett.** **101**, 239702, 2008.

[9] Lucian A. Constantin, John P. Perdew, and J. M. Pitarke, *Collapse of the Electron Gas to Two Dimensions in Density Functional Theory*, **Phys. Rev. Lett.** **101**, 016406, 2008; (E) **Phys. Rev. Lett.** **108**, 269902, 2008.

[8] John P. Perdew, Adrienn Ruzsinszky, Gábor I. Csonka, Oleg A. Vydrov, Gustavo E. Scuseria, Lucian A.



Constantin, Xiaolan Zhou, and Kieron Burke, *Restoring the Density-Gradient Expansion for Exchange in Solids and Surfaces*, **Phys. Rev. Lett.** **100**, 136406, 2008; (E) **Phys. Rev. Lett.** **102**, 039902, 2009.

[7] Lucian A. Constantin, J. M. Pitarke, J. F. Dobson, A. Garcia-Lekue, and John P. Perdew, *High-Level Correlated Approach to the Jellium Surface Energy, without Uniform-Gas Input*, **Phys. Rev. Lett.** **100**, 036401, 2008.

[6] Lucian A. Constantin, *Dimensional crossover of the exchange-correlation energy at the semilocal level*, **Phys. Rev. B** **78**, 155106, 2008.

[5] John P. Perdew and Lucian A. Constantin, *Laplacian-level density functionals for the kinetic energy and exchange-correlation energy*, **Phys. Rev. B** **75**, 155109, 2007.

[4] Lucian A. Constantin, and J.M. Pitarke, *Simple, dynamic exchange-correlation kernel of a uniform electron gas*, **Phys. Rev. B** **75**, 245127, 2007.

[3] John P. Perdew, Lucian A. Constantin, Espen Sagvolden, and Kieron Burke, *Relevance of Slowly Varying Electron Gas to Atoms, Molecules, and Solids*, **Phys. Rev. Lett.** **97**, 223002, 2006.

[2] J. M. Pitarke, Lucian A. Constantin, and John P. Perdew, *Wave-vector analysis of the jellium exchange-correlation surface energy in the random-phase approximation: Support for nonempirical density functionals*, **Phys. Rev. B** **74**, 045121, 2006.

[1] Lucian A. Constantin, John P. Perdew, and Jianmin Tao, *Meta-generalized gradient approximation for the exchange-correlation hole with an application to the jellium surface energy*, **Phys. Rev. B** **73**, 205104, 2006.

Date: April 08, 2020;

Signature: Lucian A. Constantin

