

Dr. Santiago Aparicio-Martínez

Nationality: Spanish

Current position: Professor of Physical Chemistry (Tenured). Department of Chemistry. University of Burgos. Spain.

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EDUCATION

- Ph. D. in Physical Chemistry. University of Burgos. Spain. 2001.
 - M. Sc. in Physical Chemistry. Dublin City University. Ireland. 1996.
 - M. Sc. in Physical Chemistry. University of Burgos. Spain. 1996.
 - B. Sc. in Chemistry. University of Valladolid. Spain. 1995.
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POSITIONS

- **Professor (tenured).** Department of Chemistry. University of Burgos. Spain. 2009 to date.
 - **Associate Professor.** Department of Chemistry. University of Burgos. Spain. 2006-2009.
 - **Visiting Fulbright Scholar.** Department of Chemical Engineering. Texas A&M University. USA. 2005-2006.
 - **Assistant Professor.** Department of Chemistry. University of Burgos. Spain. 1998-2005.
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RESEARCH LINES

- Molecular modelling of complex materials.
 - CO₂ capture.
 - Methane storage.
 - Ionic liquids.
 - Deep eutectic solvents.
 - 2D materials.
 - Natural gas science and technology.
 - Natural gas hydrates.
 - Carbon nanomaterials.
 - Thermophysics of complex materials.
 - Green solvents.
 - Ionanofluids.
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PHD THESIS DIRECTOR (last five years)

- Title: Methane Storage by Porous Nanocomposites of Ionic Liquids.
Student: Alberto Gutiérrez. Under development.
 - Title: A Theoretical Study of 2D Novel Solid Lubricants
Student: Loukia Maritsa. Under development.
 - Title: Design and Characterization of Porous Liquids for CO₂ Capture and Gas Separation
Student: Claudia Pecoraro. Under development.
 - Title: On the Suitability of Ionic Liquids for Environmental Applications: a Computational Study.
Student: Cesar Herrera. Under development.
 - Title: Effect of application of municipal waste compost and other organic amendments on crop production. Student: M^a Antonieta Monge. Summa cum Laude.
 - Title: Thermophysical properties of pyrrolidone based systems. Student: M.J. Dávila. Summa cum Laude.
 - Title: On the behavior of alkylbenzoate based complex fluids. Student: M. Navarro. Summa cum Laude.
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ADMINISTRATIVE POSITIONS

- Member of the University of Burgos Government Board. 2000-2004.
 - Member of the University of Burgos Research Board. 2000-2004.
 - Member of the University of Burgos Personnel board. 2003-2006 and 2011 to date.
 - Coordinator of studies in the Bachelor of Science in Chemistry. 2006 – 2009.
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MEMBER OF JOURNAL EDITORIAL BOARDS

- Advances in Materials Science Journal (Publisher: Hindawi). Member of the Editorial Board from 2010 to date.
 - Physical Chemistry Journal (Publisher: Scientific and Academic Publishing, USA). Editor-in-Chief, from 2012 to date.
 - Journal of Physics and Astronomy (Publisher: Mehta Press). Member of the Editorial Board from 2010 to date.
 - International Journal of Liquid State Sciences (Publisher: Serial Publications). Member of the Editorial Board from 2008 to date.
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JOURNAL REVIEWER

- Nature Communications.
 - Journal of Physical Chemistry A/B/C(Publisher: American Chemical Society).
 - Chemical Engineering Science (Publisher: Elsevier).
 - Journal of Molecular Modelling (Publisher: Springer).
 - Industrial and Engineering Chemistry Research (Publisher: American Chemical Society).
 - Energy and Fuels (Publisher: American Chemical Society).
 - Journal of Chemical and Engineering Data (Publisher: American Chemical Society).
 - Physical Chemistry Chemical Physics (Publisher: Royal Society of Chemistry).
 - Green Chemistry (Publisher: Royal Society of Chemistry).
 - Fluid Phase Equilibria (Publisher: Elsevier).
 - Journal of Molecular Liquids (Publisher: Elsevier).
 - Chemical Physics Letters (Publisher: Elsevier).
 - Thermochimica Acta (Publisher: Elsevier).
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INSTITUTIONAL REVIEWER

- External reviewer for National Institute of Standard and Technology (USA). Reviewing proposals.
 - International reviewer for Portugal National Science Agency. Reviewer for project proposals.
 - International reviewer for Austrian Science Fund. Reviewer for project proposals.
 - International reviewer for Argentinian Science Agency. Reviewer for project proposals.
 - International reviewer for Denmark Science Agency. Reviewer for project proposals.
 - International reviewer for Poland Science Agency. Reviewer for project proposals.
 - Reviewer for Spanish Ministry of Science. Reviewer for project proposals.
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RESEARCH FUNDING

The most relevant grants for last five years are:

- Project Title: Solid lubrication for emerging engineering applications (SOLUTION). Funding Agency: European Commission (H2020-MSCA-ITN-2016), 2017-2021. Funding: 3 510 527 Euros.
- Project: CO₂ absorbing Materials (CO2MPRISE). Funding Agency: European Commission (H2020-MSCA-RISE-2016-CO2MPRISE-734873), 2017-2021. Funding: 702 000 Euros.
- Project: Setting an interdisciplinary/sectorial/international research network to explore dry storage as an alternative strategy for cells/germplasm biobanking (DRYNET). Funding Agency: European Commission (H2020-MSCA-RISE-2016-DRYNET-734434), 2017-2021. Funding: 841 500 Euros.

- Project Title: Acid Gas Removal by Ionic Liquids: an Experimental and Computational Approach. Funding Agency: Spanish Ministry of Economy, 2014-2017. Funding: 60,000 Euros.
- Project Title: Postcombustion CO₂ Capture by Ionic Liquids. Funding Agency: Government of Castile and Leon, 2014 – 2016. Funding: 37,000 Euros.
- Project title: A computational study on ionanofluids. Funding Agency: Spanish Ministry of Science Fund. 2013-2015. Funding: 50,000 Euros.
- Project title: Avoiding Gas Hydrate Problems in Qatari's Oil and Gas Industry: An Integrated Experimental and Modeling Approach. Funding Agency: Qatar National Research Fund. 2013-2016. Funding: 1,048,000 \$.
- Project title: Natural Gas Hydrates. Funding Agency: Department of Energy USA, for National Energy Scientific Computing (NERSC) Facility. 2012. Funding: 100,000 hours of computing at NERSC facilities.
- Project title: Ionic liquids for CO₂ capture. Funding Agency: Spanish Ministry of Science. 2010-2011. Funding: 181,500 Euros.
- Project title: Measurement of Densities and Phase Envelopes for Qatari Type Natural Gas Mixtures and Developments of a Rational Equation of State to Describe the Data. Funding Agency: Qatar National Research Fund. 2008-2011. Funding: 750,000 \$.
- Project title: Design of new families of Ionic liquids for CO₂ capture. Funding Agency: University of Burgos. 2010. Funding: 30,000 Euros.
- Project title: Thermophysical Properties of Non-halogenated Ionic Liquids. Funding Agency: Spanish Ministry of Science. 2005-2008. Funded: 89,250 Euros.

PUBLICATIONS LIST (h-index = 30, i-index = 80, Total citations = 3261)

- 158.- Herrera, C.; Atilhan, M.; Aparicio, S.
A Theoretical Study on Mixtures of Amino Acid-Based Ionic Liquids
(2018) *Physical Chemistry Chemical Physics*, 20, 10213-10223.
- 157.- Aparicio, S.; Yavuz, C. T.; Atilhan, M.
Molecular Insights into Benzimidazole-linked Polymer Interactions with Carbon Dioxide and Nitrogen
(2018) *Chemistry Select*, 3, 3691-3701.
- 156.- Altamash, T.; Nasser, M. S.; Elhamarnah, Y.; Magzoub, M.; Ullah, R.; Qiblawey, H.; Aparicio, S.; Atilhan, M.
Gas solubility and rheological behavior study of betaine and alanine based natural deep eutectic solvents (NADES)
(2018) *Journal of Molecular Liquids* 256, pp. 286-295
- 155.- Gutiérrez, A.; Atilhan, M.; Alcalde, R.; Trenzado, J. L. Aparicio, S.
Insights on the mixtures of imidazolium based ionic liquids with molecular solvents
(2018) *Journal of Molecular Liquids* 255, pp.199-207.
- 154.- Alcalde, R.; Atilhan, M.; Aparicio, S.
Intermolecular forces in 1-butyl-3-methylimidazolium bis (trifluoromethylsulfonyl) imide+ ethanol mixtures
(2018) *Journal of Molecular Liquids*, 258, pp. 1-9.
- 153.- Gutiérrez, A.; Atilhan, M.; Aparicio, S.
Molecular Modeling Analysis of CO₂ Absorption by Glymes
(2018) *Journal of Physical Chemistry B*, 122, pp. 1948-1957.
- 152.- Herrera, C.; Alcalde, R.; Atilhan, M.; Aparicio, S.
Microscopic characterization of mixtures of amino acid ionic liquids and organic solvents
(2018) *Journal of Molecular Liquids* 250, pp. 111-120.
- 151.- Atilhan, M.; Aparicio, S.
Theoretical Study of Low Viscous Ionic Liquids at the Graphene Interface
(2018) *Journal of Physical Chemistry C*. 122, pp. 1645-1656.
- 150.- Ullah, R., Ali H Salah Saad, M., Aparicio, S., Atilhan, M.
Adsorption equilibrium studies of CO₂, CH₄ and N₂ on various modified zeolites at high pressures up to 200 bars
(2018) *Microporous and Mesoporous Materials*, 262, pp. 49-58.

- 149.- Herrera, C., Alcalde, R., Atilhan, M., Aparicio, S.
Microscopic characterization of mixtures of amino acid ionic liquids and organic solvents
(2018) *Journal of Molecular Liquids*, 250, pp. 111-120.
- 148.- Gutiérrez, A., Atilhan, M., Aparicio, S.
A nanoscopic approach on benzene-toluene-xylenes extraction by sulfolane
(2018) *Journal of Molecular Liquids*, 249, pp. 1039-1046.
- 147.- Hosseini, S.M., Alavianmehr, M.M., Gutiérrez, A., Khalifeh, R., Moghadasi, J., Aparicio, S.
On the properties and structure of 2-hydroxyethylammonium formate ionic liquid
(2018) *Journal of Molecular Liquids*, 249, pp. 233-244.
- 146.- Atilhan, M., Costa, L.T., Aparicio, S.
On the behaviour of aqueous solutions of deep eutectic solvents at lipid biomembranes
(2017) *Journal of Molecular Liquids*, 247, pp. 116-125.
- 145.- Gutiérrez, A., Atilhan, M., Aparicio, S.
Microscopic Characterization of CO₂ and H₂S Removal by Sulfolane
(2017) *Energy and Fuels*, 31 (9), pp. 9800-9813.
- 144.- Alcalde, R., Gutiérrez, A., Atilhan, M., Trenzado, J.L., Aparicio, S.
Insights into Glycol Ether-Alkanol Mixtures from a Combined Experimental and Theoretical Approach
(2017) *Journal of Physical Chemistry B*, 121 (22), pp. 5601-5612.
- 143.- Herrera, C., Costa, L.T., Atilhan, M., Aparicio, S.
Microscopic characterization of amino acid ionic liquids - water mixtures
(2017) *Journal of Molecular Liquids*, 236, pp. 81-92.
- 142.- Atilhan, M., Costa, L.T., Aparicio, S.
Elucidating the Properties of Graphene-Deep Eutectic Solvents Interface
(2017) *Langmuir*, 33 (21), pp. 5154-5165.
- 141.- Altamash, T., Haimour, T.S., Tarsad, M.A., Anaya, B., Ali, M.H., Aparicio, S., Atilhan, M.
Carbon Dioxide Solubility in Phosphonium-, Ammonium-, Sulfonyl-, and Pyrrolidinium-Based Ionic Liquids and their Mixtures at Moderate Pressures up to 10 bar
(2017) *Journal of Chemical and Engineering Data*, 62 (4), pp. 1310-1317.
- 140.- Altamash, T., Atilhan, M., Aliyan, A., Ullah, R., Nasser, M., Aparicio, S.
Rheological, Thermodynamic, and Gas Solubility Properties of Phenylacetic Acid-Based Deep Eutectic Solvents
(2017) *Chemical Engineering and Technology*, 40 (4), pp. 778-790.
- 139.- Lourenço, T.C., Aparicio, S., Costa, G.C., Costa, L.T.
Local environment structure and dynamics of CO₂ in the 1-ethyl-3-methylimidazolium bis(trifluoromethanesulfonyl)imide and related ionic liquids
(2017) *Journal of Chemical Physics*, 146 (10), art. no. 104502, .
- 138.- Atilhan, M., Aparicio, S.
Behavior of deep eutectic solvents under external electric fields: A molecular dynamics approach
(2017) *Journal of Physical Chemistry B*, 121 (1), pp. 221-232.
- 137.- García, G., Atilhan, M., Aparicio, S.
Simultaneous CO₂ and SO₂ capture by using ionic liquids: A theoretical approach
(2017) *Physical Chemistry Chemical Physics*, 19 (7), pp. 5411-5422.
- 136.- Herrera, C., de Carvalho Costa, G., Atilhan, M., Costa, L.T., Aparicio, S.
A theoretical study on aminoacid-based ionic liquids with acid gases and water
(2017) *Journal of Molecular Liquids*, 225, pp. 347-356.

- 135.- Mohamed, N.A., Tariq, M., Atilhan, M., Khraisheh, M., Rooney, D., Garcia, G., Aparicio, S.
Investigation of the performance of biocompatible gas hydrate inhibitors via combined experimental and DFT methods
(2017) *Journal of Chemical Thermodynamics*, 111, pp. 7-19.
- 134.- Qureshi, M.F., Atilhan, M., Altamash, T., Aparicio, S., Aminnaji, M., Tohidi, B.
High-pressure gas hydrate autoclave hydraulic experiments and scale-up modeling on the effect of stirring RPM effect
(2017) *Journal of Natural Gas Science and Engineering*, 38, pp. 50-58.
- 133.- Altamash, T., Qureshi, M.F., Aparicio, S., Aminnaji, M., Tohidi, B., Atilhan, M.
Gas hydrates inhibition via combined biomolecules and synergistic materials at wide process conditions
(2017) *Journal of Natural Gas Science and Engineering*, 46, pp. 873-883.
- 132.- Atilhan, M., Aparicio, S.
Properties of Dialkylcarbonate + 1-Alkanol Mixtures at the Vacuum Interface
(2016) *Journal of Physical Chemistry C*, 120 (51), pp. 29126-29134.
- 131.- Ullah, R., Atilhan, M., Anaya, B., Al-Muhtaseb, S., Aparicio, S., Patel, H., Thirion, D., Yavuz, C.T.
Investigation of Ester- and Amide-Linker-Based Porous Organic Polymers for Carbon Dioxide Capture and Separation at Wide Temperatures and Pressures
(2016) *ACS Applied Materials and Interfaces*, 8 (32), pp. 20772-20785.
- 130.- Alcalde, R., Atilhan, M., Aparicio, S.
Insights on 1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide + ethanol liquid mixtures: A molecular dynamics approach
(2016) *Journal of Chemical and Engineering Data*, 61 (8), pp. 2729-2737.
- 129.- Atilhan, M., Anaya, B., Ullah, R., Costa, L.T., Aparicio, S.
Double Salt Ionic Liquids Based on Ammonium Cations and Their Application for CO₂ Capture
(2016) *Journal of Physical Chemistry C*, 120 (31), pp. 17829-17844.
- 128.- Herrera, C., García, G., Alcalde, R., Atilhan, M., Aparicio, S.
Interfacial properties of 1-ethyl-3-methylimidazolium glycinate ionic liquid regarding CO₂, SO₂ and water from molecular dynamics
(2016) *Journal of Molecular Liquids*, 220, pp. 910-917.
- 127.- Alcalde, R., Atilhan, M., Trenzado, J.L., Aparicio, S.
Physicochemical Insights on Alkylcarbonate-Alkanol Solutions
(2016) *Journal of Physical Chemistry B*, 120 (22), pp. 5015-5028.
- 126.- Atilhan, M., Aparicio, S.
Deep eutectic solvents on the surface of face centered cubic metals
(2016) *Journal of Physical Chemistry C*, 120 (19), pp. 10400-10409.
- 125.- Qureshi, M.F., Atilhan, M., Altamash, T., Tariq, M., Khraisheh, M., Aparicio, S., Tohidi, B.
Gas Hydrate Prevention and Flow Assurance by Using Mixtures of Ionic Liquids and Synergent Compounds: Combined Kinetics and Thermodynamic Approach
(2016) *Energy and Fuels*, 30 (4), pp. 3541-3548.
- 124.- Tariq, M., Atilhan, M., Khraisheh, M., Othman, E., Castier, M., García, G., Aparicio, S., Tohidi, B.
Experimental and DFT Approach on the Determination of Natural Gas Hydrate Equilibrium with the Use of Excess N₂ and Choline Chloride Ionic Liquid as an Inhibitor
(2016) *Energy and Fuels*, 30 (4), pp. 2821-2832.
- 123.- Ullah, R., Atilhan, M., Diab, A., Deniz, E., Aparicio, S., Yavuz, C.T.
Synthesis, characterization and evaluation of porous polybenzimidazole materials for CO₂ adsorption at high pressures
(2016) *Adsorption*, 22 (2), pp. 247-260.

- 122.- Herrera, C., García, G., Atilhan, M., Aparicio, S.
A molecular dynamics study on aminoacid-based ionic liquids
(2016) *Journal of Molecular Liquids*, 213, pp. 201-212.
- 121.- García, G., Atilhan, M., Aparicio, S.
Flavonol-carbon nanostructure hybrid systems: A DFT study on the interaction mechanism and UV/Vis features
(2016) *Physical Chemistry Chemical Physics*, 18 (6), pp. 4760-4771.
- 120.- Atilhan, M., Ullah, R., Aparicio, S., Patel, H., Yavuz, C.T.
Comparative study on low and high pressure CO₂ adsorption capacity of organic materials
(2016) *International Congress on Energy 2016, ICE 2016 - Topical Conference at the 2016 AIChE Annual Meeting*, 2, pp. 920-926.
- 119.- Altamash, T., Atilhan, M., Aliyan, A., Ullah, R., García, G., Aparicio, S.
Insights into choline chloride-phenylacetic acid deep eutectic solvent for CO₂ absorption
(2016) *RSC Advances*, 6 (110), pp. 109201-109210.
- 118.- Ullah, R., Atilhan, M., Anaya, B., Al-Muhtaseb, S., Aparicio, S., Thirion, D., Yavuz, C.T.
High performance CO₂ filtration and sequestration by using bromomethyl benzene linked microporous networks
(2016) *RSC Advances*, 6 (70), pp. 66324-66335.
- 117.- García, G., Atilhan, M., Aparicio, S.
Interfacial Properties of Double Salt Ionic Liquids: A Molecular Dynamics Study
(2015) *Journal of Physical Chemistry C*, 119 (51), pp. 28405-28416.
- 116.- Herrera, C., Alcalde, R., García, G., Atilhan, M., Aparicio, S.
Theoretical Study of Amino Acid-Based Ionic Liquids Interacting with Carbon Nanosystems
(2015) *Journal of Physical Chemistry C*, 119 (48), pp. 27080-27094.
- 115.- García, G., Atilhan, M., Aparicio, S.
In silico rational design of ionic liquids for the exfoliation and dispersion of boron nitride nanosheets
(2015) *Physical Chemistry Chemical Physics*, 18 (2), pp. 1212-1224.
- 114.- Herrera, C., García, G., Atilhan, M., Aparicio, S.
A molecular dynamics study on aminoacid - based ionic liquids
(2016) *Journal of Molecular Liquids*, 213, 201-212.
- 113.- Alcalde, R., García, G., Atilhan, M., Aparicio, S.
Systematic Study on the Viscosity of Ionic Liquids: Measurement and Prediction
(2015) *Industrial and Engineering Chemistry Research*, 54, 10918-10924.
- 112.- Ullah, R., Atilhan, M., Aparicio, S., Canlier, A., Yavuz, C. T.
Insights of CO₂ adsorption performance of amine impregnated mesoporous silica (SBA-15) at wide range pressure and temperature conditions
(2015) *International Journal of Greenhouse Gas Control*, 43, 22-32.
- 111.- García, G., Atilhan, M., Aparicio, S.
Nanowetting of Graphene by Ionic Liquid Droplets
(2015) *Journal of Physical Chemistry C*, 119, 24529-24537.
- 110.- García, G., Atilhan, M., Aparicio, S.
The impact of charges in force field parameterization for molecular dynamics simulations of deep eutectic solvents
(2015) *Journal of Molecular Liquids*, 211, 506-514.
- 109.- García, G., Atilhan, M., Aparicio, S.
Interaction Mechanism Insights on the Solvation of Fullerene B80 with Choline-based Ionic Liquids
(2015) *Journal of Physical Chemistry B*, 119, 12455-12463.
- 108.- García, G., Atilhan, M., Aparicio, S.
Interfacial Properties of Deep Eutectic Solvents Regarding to CO₂ Capture
(2015) *Journal of Physical Chemistry C*, 119, 21413-21425.

- 107.- García, G., Atilhan, M., Aparicio, S.
Theoretical Study of Renewable Ionic Liquids in the Pure State and with Graphene and Carbon Nanotubes
(2015) Journal of Physical Chemistry B, 119, 12224-12237.
- 106.- García, G., Atilhan, M., Aparicio, S.
Theoretical Study on the Solvation of C60 Fullerene by Ionic Liquids II: DFT Analysis of the Interaction Mechanism
(2015) Journal of Physical Chemistry B, 119, 10616-10629.
- 105.- García, G., Atilhan, M., Aparicio, S.
A theoretical study on mitigation of CO₂ through advanced deep eutectic solvents
(2015) International Journal of Greenhouse Gas Control, 39, 62-73.
- 104.- García, G., Atilhan, M., Aparicio, S.
Adsorption of choline benzoate ionic liquid on graphene, silicene, germanene and boron-nitride nanosheets: a DFT perspective
(2015) Physical Chemistry Chemical Physics, 17, 16315-16326.
- 103.- García, G., Atilhan, M., Aparicio, S.
An approach for the rationalization of melting temperature for deep eutectic solvents from DFT
(2015) Chemical Physics Letters, 634, 151-155.
- 102.- García, G., Atilhan, M., Aparicio, S.
A density functional theory insight towards the rational design of ionic liquids for SO₂ capture
(2015) Physical Chemistry Chemical Physics, 17, 13559-13574.
- 101.- García, G., Atilhan, M., Aparicio, S.
Flavonols on graphene: a DFT insight
(2015) Theoretical Chemistry Accounts, 134, 13.
- 100.- García, G., Atilhan, M., Aparicio, S.
Water Effect on Acid-Gas Capture Using Choline Lactate: A DFT Insight beyond Molecule-Molecule Pair Simulations
(2015) Journal of Physical Chemistry B, 119, 5546-5557.
- 99.- Alcalde, R., García, G., Trenzado, J.L., Atilhan, M., Aparicio, S.
Characterization of Amide-Alkanediol Intermolecular Interactions
(2015) Journal of Physical Chemistry B, 119, 4725-4738.
- 98.- García, G., Aparicio, S., Atilhan, M.
Density functional theory study on the cholinium dihydrogenphosphate ionic liquid for acid gas removal
(2015) Journal of Solution Chemistry, 44, 890-899.
- 97.- Ullah, R., Atilhan, M., Anaya, B., Khraisheh, M., García, G., Elkhattat, A., Tariq, M., Aparicio, S.
A detailed study of cholinium chloride and levulinic acid deep eutectic solvent system for CO₂ capture via experimental and molecular simulation approaches
(2015) Physical Chemistry Chemical Physics, 17, 20941-20960.
- 96.- García, G., Atilhan, M., Aparicio, S.
Assessment of DFT methods for studying acid gas capture by ionic liquids
(2015) Physical Chemistry Chemical Physics, 17, 26875-26891.
- 95.- García, G., Aparicio, S., Ullah, R., Atilhan, M.
Deep eutectic solvents: Physicochemical properties and gas separation applications
(2015) Energy and Fuels, 29, 2616-2644.
- 94.- Atilhan, M.; Aparicio, S.; Ejaz, S.; Zhou, J.; Al-Marri, M.; Holste, J. J.; Hall, K. R.
Thermodynamic Characterization of Deepwater Natural Gas Mixtures with Heavy Hydrocarbon Content at High Pressures
(2015) Journal of Chemical Thermodynamics, 82, 134- 142.

- 93.- Tariq, M.; Rooney, D.; Othman, E.; Aparicio, S.; Atilhan, M., Khraisheh, M.
Gas Hydrate Inhibition: A Review of the Role of Ionic Liquids
(2014) *Industrial and Engineering Chemistry Research*, 53, 17855-17868.
- 92.- García, G.; Atilhan, M.; Aparicio, S.
Theoretical Study on the Solvation of C60 Fullerene by Ionic Liquids
(2014) *Journal of Physical Chemistry B* 118, 11330-11340.
- 91.- García, G.; Trenzado, J. L.; Alcalde, R.; Rodríguez, A.; Atilhan, M.; Aparicio, S.
Structure of Alkylcarbonate + n-Alkane Mixed Fluids
(2014) *Journal of Physical Chemistry B* 118, 11310-11322.
- 90.- García, G.; Atilhan, M.; Aparicio, S.
Insights into alkyl lactate + water mixed fluids
(2014) *Journal of Molecular Liquids* 199, 215-223.
- 89.- García, G.; Atilhan, M.; Aparicio, S.
A theoretical study on ionic liquid endohedral C540 fullerene
(2014) *RSC Advances* 4, 45826-45299.
- 88.- Atilhan, M.; Aparicio, S.
Folding of Graphene Nanostructures Driven by Ionic Liquids Nanodroplets
(2014) *Journal of Physical Chemistry C* 118, 21081-21091.
- 87.- García, G.; Atilhan, M.; Aparicio, S.
Viscous origin of ionic liquids at the molecular level: A quantumchemical insight
(2014) *Chemical Physics Letters* 610-611, 267-272.
- 86.- Herrera, C.; Alcalde, R.; Atilhan, M.; Aparicio, S.
Theoretical Study on Amino Acid-Based Ionic Pairs and Their Interaction with Carbon Nanostructures
(2014) *Journal of Physical Chemistry C* 118, 9741-9757.
- 85.- Atilhan, M.; Pala, N., Aparicio, S.
A quantum chemistry study of natural gas hydrates
(2014) *Journal of Molecular Modeling* 20, 2182.
- 84.- Sanz, V.; Alcalde, R.; Atilhan, M.; Aparicio, S.
Insights from quantum chemistry into piperazine-based ionic liquids and their behavior with regard to CO₂
(2014) *Journal of Molecular Modeling* 20, 2107.
- 83.- Aparicio, S.; Atilhan, M.; Pala, N.
Insights on cholinium- and piperazinium-based ionic liquids under external electric fields: A molecular dynamics study
(2013) *Journal of Chemical Physics* 139, 224502.
- 82.- Atilhan, M.; Jacquemin, J., Rooney, D.; Khraisheh, M.; Aparicio, S.
Viscous Behavior of Imidazolium-Based Ionic Liquids
(2013) *Industrial and Engineering Chemistry Research* 52, 16774-16785.
- 81.- Aparicio, S., Atilhan, M.
Molecular Dynamics Study of Carbon Nanostructures in N-Methylpiperazinium Lactate Ionic Liquid
(2013) *Journal of Physical Chemistry C* 117, 22046-22059.
- 80.- Jung, J. Y.; Karadas, F.; Zulfqar, S.; Deniz, E.; Aparicio, S.; Atilhan, M.; Yavuz, C. T.; Han, S. N.
Limitations and high pressure behavior of MOF-5 for CO₂ capture
(2013) *Physical Chemistry Chemical Physics* 15, 14319-14327.
- 79.- Aparicio, S.; Atilhan, M.
On the Properties of CO₂ and Flue Gas at the Piperazinium-Based Ionic Liquids Interface: A Molecular Dynamics Study
(2013) *Journal of Physical Chemistry C* 117, 15061-15074.

- 78- Aparicio, S.; Atilhan, M.
Nanoscopic Vision on Fuel Dearomatization Using Ionic Liquids: The Case of Piperazine-Based Fluids
(2013) *Energy and Fuels* 2515-2527.
- 77.- Deniz, E.; Karadas, F.; Patel, H. A.; Aparicio, S., Yavuz, C. T., Atilhan, M.
A combined computational and experimental study of high pressure and supercritical CO₂ adsorption on Basolite MOFs
(2013) *Microporous and Mesoporous Materials* 175, 34-42.
- 76.- Caro, M.; Trenzado, J. L.; Galván, S.; Romano, E.; González, E.; Alcalde, R.; Aparicio, S.
Densities and Viscosities of Three Binary Monoglyme + 1-Alcohol Systems from (283.15 to 313.15) K
(2013) *Journal of Chemical and Engineering Data* 58, 909-914.
- 75- Karadas, F., Koz, B., Jacquemin, J., Deniz, E., Rooney, D., Thompson, J., Yavuz, C.T., Khraisheh, M., Aparicio, S., Atilhan M.
High pressure CO₂ absorption studies on imidazolium based ionic liquids: experimental and simulation approaches
(2013) *Fluid Phase Equilibria*, 351, 74-86.
- 74- Atilhan, M., Aparicio, S.
ProT measurements and derived properties of liquid 1,2-alkanediols
(2012) *Journal of Chemical Thermodynamics*, 57, 137-144.
- 73- Atilhan, M., Aparicio, S.
Review on natural gas thermophysical property measurement techniques
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