Curriculum Vitae

Name: **Miguel Ángel Soler**

Date: May 7, 2017

Surname: Soler First name: Miguel Ángel
Researcher unique identifier(s): Researcher ID J-2389-2013 ORCID code: 0000-0002-5780-9949
URL for web site: http://www.researchgate.net/profile/Miguel_Soler/
https://scholar.google.com/citations?hl=en&user=4zg2WxMAAAAJ
ID Number: 48501415 Date of birth: November 11, 1982 Sex: M

Academic position

Center: Scuola Internazionale Superiore di Studi Avanzati (SISSA)
Group: Molecular and Statistical Biophysics group.
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Specialization (UNESCO code): 2406, 2210, 2302.24, 2302.26, 2302.27
Academic Position: Posdoctoral Fellow Date: July 1, 2016 -

Reserach lines

Protein molecular recognition, protein folding, peptides and proteins, vibrational energy in solution, molecular dynamics, Monte Carlo.

Education

Bachelor	Center	Date
Chemistry	Faculty of Chemistry. University of Murcia	September 30, 2005

Advance Studies Degree	Center	Date
Physical Chemistry	Faculty of Chemistry. University of Murcia	December 12, 2007

Ph.D.	Center	Date
Chemistry	Faculty of Chemistry. University of Murcia	June 15, 2010

Professional Experience

Position	Institution	Date
Posdoctoral Fellow	University of Udine (Italy)	January 1, 2014 - June 30, 2016
Posdoctoral Fellow	University of Lisbon (Portugal)	October 1, 2011 - November 30, 2013
Posdoctoral Fellow	University of Quilmes (Argentina)	April 1, 2011 - September 30, 2011
Posdoctoral Research Associate	University of Murcia (Spain)	June 15, 2010 - April 1, 2011
Graduate Research Assistant	University of Murcia (Spain)	January 1, 2007 - June 15, 2010

Languages (R=regular, G=good ,C=correct)

Language	Speaking	Reading	Writting
Spanish	C	C	C
English	C	C	C
Italian	C	C	C
Portuguese	C	C	C
German	R	R	R

Research Experience

My PhD thesis in Murcia (Spain) focused on the multiscale simulation of the vibrational relaxation of peptides in liquid solvents, exploring a wide range of simulations techniques, such as molecular dynamics, hybrid quantum/classical perturbative treatments and hybrid quantum/classical simulations. Afterwards, motivated by expanding my knowledge in biological systems and additional computational approaches I moved to Lisbon (Portugal) to work as postdoc in the protein folding field. There, I developed coarse grained models to study how proteins with physical knots are able to fold into their native structure. At the beginning of 2014, I came to Italy to work, first in the Scoles' group in Udine and now in the Laio's group in SISSA (Trieste), in a multidisciplinary approach for the design of peptides as probes for the molecular recognition of protein biomarkers.

I keep currently the collaboration with some of my former supervisors: Profs. Bastida (Spain), Fernández-Alberti (Argentina), and Faísca (Portugal), with whom I have published recently, or I will do during this year, several articles. Furthermore, I have taken advantage of the multidisciplinary environment that offers my current research group to stablish collaborations with other scientists and research groups of the local area. Profs. Fogolari (Univ. Udine) in the theoretical/computational field, and Profs. de Marco (Univ. Nova Gorica), and Corazza (Univ. Udine) in the experimental field, are some important examples of my actual collaborations.

I+D Projects (last 10 years)

1. **Title of the Project**: Application of Advanced Nanotechnology in the Development of Cancer Diagnostics Tools (RIF. 12214).
   Funding Institutuion: Associazione Italiana per la Ricerca sul Cancro (AIRC) 5xMILLE
   From: 2011 **to**: 2017
   Funding amount: 6224670 euros
   Project leader: Giuseppe Toffoli
   Number of investigators: -

2. **Title of the Project**: Molecular Nanotechnology for Life Science Applications: QUantitative Interactomics for Diagnostics, PROteomics and QUantitative Oncology (ERC-2010-AdG_20100317/269051)
   Funding Institutuion: FP7-IDEAS-ERC
   From: 2011 **to**: 2016
   Funding amount: 2979700 euros
   Project leader: Giacinto Scoles
   Number of investigators: -

3. **Title of the Project**: Insights into folding kinetics and designability of knotted proteins from lattice models (PTDC/QUI-QUI/112358/2009)
   Funding Institutuion: Fundação para a Ciência e a Tecnologia
   From: 2011 **to**: 2013
   Funding amount: 70000 euros
   Project leader: Patricia Faísca
   Number of investigators: 4

4. **Title of the Project**: Relajación y redistribución intramolecular de energía vibracional en moléculas con enlaces de tipo peptídico (CTQ2007-66528)
   Funding Institutuion: Dirección General de Investigación. Ministerio de Educación y Ciencia
   From: 01/10/2007 **to**: 30/09/2010
   Funding amount: 60500 euros
   Project leader: Alberto Requena Rodríguez
   Number of investigators: 6

Fellowships and Awards

15/03/2017 – 14/09/2017	PRACE Tier 0 Type B funding project (2010PA3749) for computational resources in Hazelhen (Germany), Marconi (Italy), and Curie (France).
10/06/2014 – 10/03/2015	Class C funding project for computational resources Italian SuperComputing Resource Allocation (ISCRA), CINECA, Italy.
01/04/2011 – 01/10/2011	Postdoctoral Fellowship (CONICET, Argentinian Government Fellowship) University of Quilmes, Buenos Aires, Argentina
01/01/2006 – 31/12/2009	Predoctoral Fellowship (FPU, Spanish Government Fellowship) Physical Chemistry Depart., Faculty of Chemistry, University of Murcia, Spain
01/10/2004 – 30/06/2005	Research Scholarship Organic Chemistry Dept., Faculty of Chemistry, Univ. of Murcia, Spain
01/10/2001 – 30/06/2004	Cultural Activities Scholarship University of Murcia, Spain

Teaching Activities

01/02/2010 – 30/06/2010	Assistant Professor - Experiments in Advanced Physical Chemistry, Chemistry Bachelor, University of Murcia / Spain
30/09/2009 – 01/01/2010	Assistant Professor - Experiments in Physical Chemistry and Analitical Chemistry, Chemical Engineering Bachelor, University of Murcia / Spain
30/09/2009 – 01/01/2010	Assistant Professor - Chemistry, Physics Bachelor, University of Murcia / Spain

Peer Review

28/05/2015	Peer Review for Journal of Biomolecular Structure & Dynamics
01/02/2011	Peer Review for Journal of Molecular Modeling

Publications (last 10 years)

1. **Authors**: M.A. Soler, and S. Fortuna.
   Title: Influence of Linker Flexibility on the Binding Affinity of Bidentate Binders.
   Journal: J. Phys. Chem. B. 121(16), 3918-3924 (2017).
   Code: Article.

2. **Authors**: M.A. Soler, A. Rodriguez, A. Russo, A.F. Adedeji, C.J.D. Foumthuim, C. Cantarutti, E. Ambrosetti, L. Casalis, A. Corazza, G. Scoles, D. Marasco, A. Laio, and S. Fortuna.
   Title: Computational design of cyclic peptides for the customized oriented immobilization of globular proteins.
   Journal: Phys. Chem. Chem. Phys. 19, 2740-2748 (2017).
   Code: Article.

3. **Authors**: M.A. Soler, J. Zuñiga, A. Requena, and A. Bastida
   Title: Understanding the connection between conformational changes of peptides and equilibrium thermal fluctuations.
   Journal: Phys. Chem. Chem. Phys. 19, 3459-3463 (2017).
   Code: Article.

4. **Authors**: M.A. Soler, A. De Marco, and S. Fortuna
   Title: Molecular dynamics simulations and docking enable to explore the biophysical factors controlling the yields of engineered nanobodies.
   Journal: Scientific Reports 6, 34869 (2016).
   Code: Article.

5. **Authors**: M.A. Soler, A. Rey, and P.F.N. Faísca
   Title: Steric confinement and enhanced local flexibility assist knotting in simple models of protein folding.
   Journal: Phys. Chem. Chem. Phys. 18 (38), 26391-26403 (2016).
   Code: Article.

6. **Authors**: A. Bastida, J. Zúñiga, A. Requena, B. Miguel, M.E. Candela, and M. A. Soler.
   Title: Conformational changes of trialanine in water induced by vibrational relaxation of the amide I mode.
   Journal: J. Phys. Chem. B, 120 (2), pp 348-357 (2016).
   Code: Article.

7. **Authors**: F. Fogolari, C.J.D. Foumthuim, S. Fortuna, M. A. Soler, A. Corazza, and G. Esposito.
   Title: Accurate estimation of the entropy of rotation-translation probability distributions.
   Journal: J. Chem. Theory Comput., 12 (1), pp 1-8 (2016).
   Code: Article.

8. **Authors**: M.A. Soler, S. Fortuna, G. Scoles.
   Title: Computational design of peptides as probes for the recognition of protein biomarkers.
   Journal: Eur Biophys J, 44 (Suppl 1):S149 (2015).
   Code: Abstract.

9. **Authors**: F. Fogolari, A. Corazza, S. Fortuna, M. A. Soler, B. VanSchouwen, G. Brancolini, S. Corni, G. Melacini, and G. Esposito
   Title: Distance-based configurational entropy of proteins from molecular dynamics simulations.
   Journal: PLoS ONE 10(7): e0132356. (2015).
   Code: Article.

10. **Authors**: M. A. Soler, A. Nunes and P. Faísca
    Title: Effects of knot type in the folding of topologically complex lattice proteins.
    Journal: J. Chem. Phys. 141, 025101 (2014).
    Code: Article.

11. **Authors**: M. A. Soler, T. Nelson, A. Roitberg, S. Tretiak and S. Fernández-Alberti
Title: A signature of nonadiabatic couplings in molecular excited states vibrational modes.
Journal: J. Phys. Chem. A, 118 (45), 10372-10379 (2014).
Code: Article.

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12. **Authors**: M. A. Soler and P.F.N. Faísca
Title: The effects of knots on protein folding properties.
Journal: PLoS ONE 8(9): e74755 (2013).
Code: Article.

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13. **Authors**: M. A. Soler and P.F.N. Faísca
Title: Understanding the effects of knots on protein folding properties.
Journal: Protein Science, 22, Issue S1, 96-97 (2013).
Code: Abstract.

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14. **Authors**: M. A. Soler and P.F.N. Faísca
Title: How Difficult Is It to Fold a Knotted Protein? In Silico Insights from Surface-Tethered Folding Experiments.
Journal: PLoS ONE 7(12): e52343 (2012).
Code: Article.

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15. **Authors**: M. A. Soler, A. Roitberg, T. Nelson, S. Tretiak and S. Fernández-Alberti
Title: Analysis of state-specific vibrations coupled to the unidirectional energy transfer in conjugated dendrimers
Journal: J. Phys. Chem. A, 116, 9802-9810 (2012).
Code: Article.

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16. **Authors**: A. Bastida, M. A. Soler, J. Zúñiga, A. Requena, A. Kalstein and S. Fernández-Alberti.
Title: Hybrid Quantum/Classical Simulations of the Vibrational Relaxation of the Amide I Mode of N-Methylacetamide in D2O Solution
Journal: J. Phys. Chem. B, 116, 2969-2980 (2012).
Code: Article.

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17. **Authors**: M. A. Soler, A. Bastida, M. H. Farag, J. Zúñiga and A. Requena.
Title: A method for analyzing the vibrational energy flow in biomolecules in solution.
Journal: J. Chem. Phys., 135, 204106 (2011).
Code: Article.

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18. **Authors**: A. Kalstein, S. Fernández-Alberti, A. Bastida, M. A. Soler, M. H. Farag, J. Zúñiga and A. Requena.
Title: Vibrational dynamics of polyatomic molecules in solution: assignment, time evolution and mixing of instantaneous normal modes.
Journal: Theor. Chem. Acc. 128, 769-782 (2011).
Code: Article.

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19. **Authors**: A. Bastida, M. A. Soler, J. Zúñiga, A. Requena, A. Kalstein and S. Fernández-Alberti.
Title: Molecular dynamics simulations and instantaneous normal mode analysis of the vibrational relaxation of the C-H stretching modes of N-methylacetamide-D in liquid deuterated water.
Journal: J. Phys. Chem. A, 114, 11450-11461 (2010).
Code: Article.

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20. **Authors**: A. Bastida, M. A. Soler, J. Zúñiga, A. Requena, A. Kalstein and S. Fernández-Alberti.
Title: Instantaneous normal modes, resonances. and decay channels in the vibrational relaxation of the amide I mode of N-methylacetamide-D in liquid deuterated water.
Journal: J. Chem. Phys., 132, 224501 (2010).
Code: Article.

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21. **Authors**: A. Bastida, M. A. Soler, J. Zúñiga, A. Requena and B. Miguel.
Title: Efficient parabolic evaluation of coupling terms in hybrid quantum/classical simulations.
Journal: Chem. Phys, 358, 57-60 (2009).
Code: Article.

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22. **Authors**: A. Espinosa, A. Frontera, R. García, M. A. Soler and A. Tárraga.
Title: Electrophilic behavior of 3-methyl-2-methylthio-1,3,4-thiadiazolium salts: a multimodal theorical approach.
Journal: ARKIVOC, IX, 415-437 (2005).
Code: Article.

Congress and others Cientifical Meetings

1. **Authors**: Miguel A. Soler, and Sara Fortuna.
   Title: Computational design of nanobodies for the molecular recognition of protein targets.
   Participation rate: Oral presentation.
   Congress: Self-assembly, Recognition and Applications, Institute of Physics (IOP).
   Place: Edinburgh, UK. **Date**: December 9, 2016.

2. **Authors**: Miguel A. Soler, Ario de Marco and Sara Fortuna.
   Title: Computational design of customised nanobodies for biotechnological applications.
   Participation rate: Poster.
   Congress: The Physics of Soft and Biological Matter, Institute of Physics (IOP).
   Place: Cambridge, UK. **Date**: April 6 - 8, 2016.

3. **Authors**: Miguel A. Soler, Sara Fortuna and Giacinto Scoles.
   Title: Computational design of peptides as probes for the recognition of protein biomarkers.
   Participation rate: Poster.
   Congress: 10th European Biophysics Congress.
   Place: Dresden, Germany. **Date**: July 18 - 22, 2015.

4. **Authors**: Miguel A. Soler, Sara Fortuna y Giacinto Scoles.
   Title: Computational design of peptides as probes for the recognition of Beta-2-microglobulin.
   Participation rate: Poster.
   Congress: EMBO Workshop on Advances in protein-protein interaction analysis and modulation.
   Place: Hyeres, France. **Date**: September 9 - 12, 2014.

5. **Authors**: T. Nelson, M. A. Soler, A. Roitberg, S. Tretiak, S. Fernandez-Alberti.
   Title: Signature of Nonadiabatic Coupling in Excited-State Vibrational Modes.
   Participation rate: Poster.
   Congress: APS March Meeting 2014.
   Place: Denver, Colorado (USA). **Date**: March 3 - 7, 2014.

6. **Authors**: M. A. Soler and P.F.N. Faísca.
   Title: Understanding the effects of knots on protein folding properties.
   Participation rate: Poster.
   Congress: The 27th Annual Symposium of the Protein Society.
   Place: Boston (USA). **Date**: July 20 - 23, 2013.

7. **Authors**: M. A. Soler and P.F.N. Faísca.
   Title: How difficult is it to fold a knotted protein? The effect of surface tethering.
   Participation rate: Poster.
   Congress: Workshop of Protein Folding: Integrating theory, simulation and experiment.
   Place: Zurich (Switzerland). **Date**: September 3 - 6, 2012.

8. **Authors**: A. Kalstein, M. A. Soler, A. Bastida and S. Fernández-Alberti.
   Title: Simulación híbrida clásico cuántica de la relajación vibracional del modo amida I de la N-metilacetamida en solución
   Participation rate: Poster.
   Congress: XVII Congreso Argentino de Fisicoquímica y Química Orgánica.
   Place: Córdoba (Argentina). **Date**: May 3 - 6, 2011.

9. **Authors**: A. Kalstein, M. A. Soler, A. Bastida and S. Fernández-Alberti.
   Title: Molecular Dynamics simulations using normal modes coordinates to study the vibrational energy flow through the amide group.
   Participation rate: Poster.
   Congress: VII Iberoamerican Congress of Byophysics 2009.
   Place: Buzios, Rio de Janeiro (Brazil). **Date**: September 30 - October 3, 2009.

10. **Authors**: A. Kalstein, M. A. Soler, A. Bastida and S. Fernández-Alberti.
    Title: Identificación de canales específicos de relajación y redistribución de la energía vibracional de la N-metilacetamida en solución.
    Participation rate: Poster.
    Congress: XVI Congreso Argentino de Fisicoquímica y Química Inorgánica.
    Place: Universidad Nacional de Salta, Salta (Argentina). **Date**: May 18 - 21, 2009.

11. **Meeting**: Summer School of Mixed Quantum-Classical Dynamics: Foundations and Application to Photo-Biological Questions.
Participation rate: Student.
Place: University of Vienna, Vienna (Austria). **Date**: July 7 - 12, 2008.

12. **Meeting**: European Master in Theorical Chemistry and Computational Modelling.
Participation rate: Student.
Place: Universidad Autónoma de Madrid, Madrid (Spain). **Date**: September 3 - 29, 2007.

13. **Meeting**: EARLINET-ASOS Workshop.
Participation rate: Student.
Place: Universidad de Granada, Granada (Spain). **Date**: October 9 - 11, 2006.

14. **Meeting**: Curso de Doctorado Interuniversitario en Química Teórica y Computacional.
Participation rate: Student.
Place: Universidad Rovira i Virgili, Tarragona (Spain). **Date**: January 16 - February 11, 2006.

Other merits

- Intermedium level (B1) in German.
Official Language School.
- Advanced user of the Linux and Windows OSs.
- Advanced knowledges of programming in Fortran, C++ and Bash Scripting.
- Advanced user of Gromacs, HADDOCK, Autodock Vina, FoldX, Pymol, and VMD programs.
- Advanced user of Latex, OpenOffice and Microsoft Word editors.