Co-authored publications and FP7/ H2020 proposals

Co-authored publications

Enter in the table below only publications on the topic of the Action, co-authored by at least two Action participants from two different countries participating in the Action and for which the Action networking added value. A maximum of ten publications may be entered. If the Action has more than ten such publications the Core Group should select the ten most significant ones to include in the table below.

No.	Bibliographic data (including: Title, Authors, Title of the periodical or the series, Issue number or volume, Publisher, Year of publication, Relevant pages)	Main author	Number of authors	Action participants listed among the authors (Name, country and role[1])	WGs involved in publication	Date of submission (must be after Action start date)	Expected date of publication (if not already published)	Persistent link to publicly available version of the paper (if available) or the abstract	Is/Will open access[2] provided to this publication?	Is/ will COST be cited/ acknowledged in the publication ?	Are/ will COST funds (be) implicated in this publication	Relevance to H2020 Societal Challenges[3] ?	Is it peer-reviewed?	Was the added value of the Action Networking necessary for the publication	Impact Factor (if applicable)
1	*Mechanical properties of the quasi-one-dimensional antiferromagnet Cu(en)(H 2O) 2SO4* D. Legut, R. Sýkora, U. D. Wdowik, A. Orendáčovác J. Nanosci. Nanotech (2018), in press	D. Legut	4	D. Legut, R. Sýkora, U. D. Wdowik, A. Orendáčovác		2017	2018		No	Yes	Yes		Yes		1.483
2	*Species formed during NO adsorption and NO+O2 co-adsorption on ceria: A combined FTIR and DFT study* M. Y. Mihaylov, E. Z. Ivanova, H. A. Aleksandrov, P. St. Petkov, G. N. Vayssilov, K. I. Hadjiivanov Journal of Molecular Catalysis. A, Chemical, 2018, in press	M. Y. Mihaylov	6	M. Y. Mihaylov, E. Z. Ivanova, H. A. Aleksandrov (BG, MC Member), P. St. Petkov, G. N. Vayssilov (BG, MC Member), K. I. Hadjiivanov		2017	2018		No	Yes	Yes		Yes		4.211
3	*Magnetic Compton profiles of disordered Fe0.5Ni0.5 and ordered FeNi alloys* D. Benea, J. Minár, H. Ebert, L. Chioncel Phys. Rev. B **97**, 144408 (2018)	D. Benea	4	D. Benea (RO), J. Minár(CZ, MC Member, WG1 Leader), H. Ebert (DE, Chair), L. Chioncel	WG1 WG2 WG3 WG4	19-12-2017		https://doi.org/10.1103/PhysRevB.97.144408	No	Yes	Yes		Yes		3.836
4	*Electron transmission through a steel capillary* J. B. Maljkovic, D. Borka, M. L. Rankovic, B. P. Marinkovic, A. R. Milosavljevic, C. Lemell, T. Károly Nucl. Instrum. Meth. B 423, 87-91 (2018)	J. B. Maljkovic	7	J. B. Maljkovic, D. Borka (RS), M. L. Rankovic, B. P. Marinkovic, A. R. Milosavljevic, C. Lemell, T. Károly	WG2	14-12-2017		https://doi.org/10.1016/j.nimb.2018.03.020	No	Yes	Yes		Yes		1.362
5	*Analytical modeling of electron energy loss spectroscopy of graphene: Ab initio study versus extended hydrodynamic model* T. Djordjević, I. Radovića, V. Despoja, K. Lyon, D. Borka, Z. L. Mišković Ultramicroscopy 184, 142 (2018)	T. Djordjević	6	T. Djordjević, I. Radovića, V. Despoja, K. Lyon, D. Borka (RS), Z. L. Mišković	WG2	24-05-2017		http://dx.doi.org/10.1016/j.ultramic.2017.08.014	No	Yes	Yes		Yes		2.843
6	*Determination of the ground state of an Au-supported FePc film based on the interpretation of Fe K- and L-edge x-ray*	C. R. Natoli	4	C. R. Natoli (IT), P. Krüger (JP, NNC	WG1 WG2 WG3	17-07-2017		https://doi.org/10.1103/PhysRevB.97.155139	No	Yes	Yes		Yes		3.836

1 MC Member/ MC Substitute/ MC Observer/ WG Member/ Training School Trainee/ STSM Recipient/ Other Action Participant

2 Open Access is defined as free of charge access for anyone via Internet. Please answer "yes" if the open access to the publication is already established and also if the embargo period for open access is not yet over but you intend to establish open access afterwards.

3 H2020 Societal Challenges are “Health, demographic change and wellbeing”; “Food security, sustainable agriculture and forestry, marine and maritime and inland water research, and the Bioeconomy”; “Secure, clean and efficient energy”; “Smart, green and integrated transport”; “Climate action, environment, resource efficiency and raw materials”; “Europe in a changing world - inclusive, innovative and reflective societies”; “Secure societies - protecting freedom and security of Europe and its citizens”

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	magnetic circular dichroism measurements C. R. Natoli, P. Krüger, J. Bartolomé, F. Bartolomé Phys. Rev. B 97, 155139 (2018)			Representative), J. Bartolomé, F. Bartolomé	WG4										
7	*Absolute determination of optical constants of three transition metals using reflection electron energy loss spectroscopy* H. Xu, L. H. Yang, J. Toth, K. Tokesi, B. Da, Z. J. Ding J. Appl. Phys. **123**, 043306 (2018)	H. Xu	6	H. Xu, L. H. Yang, J. Toth, K. Tokesi, B. Da, Z. J. Ding		04-11-2017		https://doi.org/10.1063/1.5012013	No	Yes	Yes		Yes		2.068
8	*1s2p Resonant Inelastic X-ray Scattering Magnetic Circular Dichroism as a probe for the local and non-local orbitals in CrO2* P. Zimmermann, N. Bouldi, M. O. J. Y. Hunault, M. Sikora, J. M. Ablett, J. P. Rueff, B. Lebert, P. Sainctavit, F. M. F. de Groot, A. Juhin Journal of Electron Spectroscopy and Related Phenomena **222**, 74-87 (2018)	P. Zimmermann	10	P. Zimmermann, M. Sikora (PL, MC Substitute), F. M. F. de Groot (NL, MC Member), A. Juhin (AT, MC Member, STSM deputy manager)	WG1 WG2 WG3 WG4 WG5	12-11-2016		https://doi.org/10.1016/j.elspec.2017.08.004	No	Yes	Yes		Yes		1.661
9	*Scaling behavior of the Compton profile of alkali metals* M. Sekania, W. H. Appelt, D. Benea, H. Ebert, D. Vollhardt, L. Chioncel Physica A-Stat. Mech. Appl. 489, 18-27(2018)	M. Sekania	6	M. Sekania, W. H. Appelt, D. Benea (RO), H. Ebert (DE, Chair), D. Vollhardt, L. Chioncel	WG1 WG2 WG3 WG4	22-11-2016		https://doi.org/10.1016/j.physa.2017.07.018							2.243
10	*Theory of L-edge spectroscopy of strongly correlated systems* J. Lüder, J. Schött, B. Brena, M. W. Haverkort, P. Thunström, O. Eriksson, B. Sanyal, I. Di Marco, Y. O. Kvashnin Phys. Rev. B **96**, 245131 (2017)	J. Lüder	9	J. Lüder, J. Schött, B. Brena (SE, MC Member, WG2 Leader), M. W. Haverkort, P. Thunström, O. Eriksson, B. Sanyal, I. Di Marco, Y. O. Kvashnin (SE)	WG1 WG2	24-06-2017		https://doi.org/10.1103/PhysRevB.96.245131	No	Yes	Yes		Yes		3.836
11	*Optical properties of titanium oxide films obtained by cathodic arc plasma deposition* V. Jokanovic, B. Colovic, A. T. Petkoska, A. Mrakovic, B. Jokanovic, M. Nenadovic, M. Ferrara, I. Nasov Plasma Science and Technology **19**, 125504 (2017)	V. Jokanovic	8	V. Jokanovic, B. Colovic, A. T. Petkoska, A. Mrakovic, B. Jokanovic, M. Nenadovic, M. Ferrara, I. Nasov		06-07-2017		https://doi.org/10.1088/2058-6272/aa8806	No	Yes	Yes		Yes		0.830
12	*Square selenene and tellurene: novel group VI elemental 2D materials with nontrivial topological properties* L. D. Xian, A. P. Paz, E. Bianco, P. M. Ajayan, A. Rubio 2D Materials **4**, 041003 (2017)	L. D. Xian	5	L. D. Xian, A. P. Paz, E. Bianco, P. M. Ajayan, A. Rubio (ES, MC Member)	WG1 WG2 WG3	09-05-2017		https://doi.org/10.1088/2053-1583/aa8418	No	Yes	Yes		Yes		6.937
13	*Iron oxide nanoparticles - In vivo/in vitro*	M.	6	M. Nedyalkova	WG1	01-02-		https://doi.org/10.1016/j.cis.2017.05.003	No	Yes	Yes		Yes		7.223

	biomedical applications and in silico studies M. Nedyalkova, B. Donkova, J. Romanova, G. Tzvetkov, S. Madurga, V. Simeonov Advances in Colloid and Interface Science **249**, 192-212 (2017)	Nedyalkova		(BG, MC Member), B. Donkova, J. Romanova, G. Tzvetkov, S. Madurga, V. Simeonov	WG2	2017									
14	*Nonadiabatic Vibrational Damping of Molecular Adsorbates: Insights into Electronic Friction and the Role of Electronic Coherence* S. P. Rittmeyer, J. Meyer, K. Reuter Phys. Rev. Lett. **119**, 176808 (2017)	S. P. Rittmeyer	3	S. P. Rittmeyer, J. Meyer, K. Reuter		13-04-2017		https://doi.org/10.1103/PhysRevLett.119.176808	No	Yes	Yes		Yes		8.462
15	*Structural transformations and adsorption properties of PtNi nanoalloy thin film electrocatalysts prepared by magnetron co-sputtering* O. Brummel, F. Waidhas, I. Khalakhan, M. Vorokhta, M. Dubau, G. Kovacs, H. A. Aleksandrov, K. M. Neyman, V. Matolin, J. Libuda Electrochimica Acta **251**, 427-441 (2017)	O. Brummel	10	O. Brummel, F. Waidhas, I. Khalakhan, M. Vorokhta, M. Dubau, G. Kovacs, H. A. Aleksandrov (BG, MC Member), K. M. Neyman, V. Matolin, J. Libuda	WG1	05-05-2017		https://doi.org/10.1016/j.electacta.2017.08.062	No	Yes	Yes		Yes		4.798
16	Ballistic spin transport in the presence of interfaces with strong spin-orbit coupling J. Borge, I. V. Tokatly Phys. Rev. B **96**, 115445 (2017)	J. Borge	2	J. Borge, I. V. Tokatly		16-06-2017		https://doi.org/10.1103/PhysRevB.96.115445	No	Yes	Yes		Yes		3.836
17	*Local vs Nonlocal States in FeTiO3 Probed with 1s2pRIXS: Implications for Photochemistry* M. O. J. Y. Hunault, W. Khan, J. Minar (DE, MC Member, WG1 Leader), T. Kroll, D. Sokaras, P. Zimmermann, M. U. Delgado-Jaime, F. M. F. de Groot Inorganic Chemistry **56**, 10882-10892 (2017)	M. O. J. Y. Hunault	8	M. O. J. Y. Hunault, W. Khan, J. Minar (DE, MC Member, WG1 Leader), T. Kroll, D. Sokaras, P. Zimmermann, M. U. Delgado-Jaime, F. M. F. de Groot (NL, MC Member)	WG1 WG2 WG3 WG4	17-04-2017		https://doi.org/10.1021/acs.inorgchem.7b00938	No	Yes	Yes		Yes		4.857
18	*Synthesis, Modeling, and Catalytic Properties of HY Zeolite-Supported Rhodium Dinitrosyl Complexes* K. Khivantsev, A. Vityuk, H. A. Aleksandrov, G. N. Vayssilov, D. Blom, O. S. Alexeev, M. D. Amiridis ACS Catalysis **7**, 5965-5982 (2017)	K. Khivantsev	7	K. Khivantsev, A. Vityuk, H. A. Aleksandrov (BG, MC Member), G. N. Vayssilov, D. Blom, O. S. Alexeev, M. D. Amiridis	WG1	17-03-2017		https://doi.org/10.1021/acscatal.7b00864	No	Yes	Yes		Yes		10.614
19	*Chemical Bond Modification upon Phase Transformation of TiO2 Nanoribbons Revealed by Nanoscale X-ray Linear Dichroism* P. Kruger, M. Sluban, P. Umek, P. Guttmann, C. Bittencourt J. Phys. Chem. C **121**, 17038-17042 (2017)	P. Kruger	5	P. Kruger (JP, NNC Representative), M. Sluban, P. Umek, P. Guttmann, C. Bittencourt	WG1 WG2	15-06-2016		https://doi.org/10.1021/acs.jpcc.7b06968	No	Yes	Yes		Yes		4.536

20	*TDDFT-Based Study on the Proton-DNA Collision* R. Seraide, M. A. Bernal, G. Brunetto, U. de Giovannini, A. Rubio J. Phys. Chem. B 121, 7276-7283 (2017)	R. Seraide	5	R. Seraide, M. A. Bernal, G. Brunetto, U. de Giovannini (ES), A. Rubio (ES, MC Member)	WG1 WG2 WG3	22-05-2016		https://doi.org/10.1021/acs.jpcb.7b04934	No	Yes	Yes		Yes		3.177
21	*Modeling Non-Equilibrium Dynamics and Saturable Absorption Induced by Free Electron Laser Radiation* K. Hatada, A. Di Cicco Appl. Sci. **7**, 814 (2017)	K. Hatada	2	K. Hatada (FR), A. Di Cicco (IT)	WG1 WG2 WG3 WG5	31-05-2017		https://doi.org/10.3390/app7080814	No	Yes	Yes		Yes		1.679
22	*Raman scattering from single WS2 nanotubes in stretched PVDF electrospun fibers* O. Grinberg, S. W. Deng, E. Zussman, T. Livneh, A. Zak Phys. Chem. Chem. Phys. **19**, 18443-18451 (2017)	O. Grinberg	5	O. Grinberg, S. W. Deng, E. Zussman, T. Livneh, A. Zak (IL, MC Member)	WG5	11-02-2017		https://doi.org/10.1039/c7cp00934h	No	Yes	Yes		Yes		4.123
23	*Optical properties of periodic systems within the current-current response framework: Pitfalls and remedies* D. Sangalli, J. A. Berger, C. Attaccalite, M. Grüning, P. Romaniello Phys. Rev. B **95**, 155203 (2017)	D. Sangalli	5	D. Sangalli (IT), J. A. Berger, C. Attaccalite, M. Grüning (UK), P. Romaniello (FR)	WG2	23-01-2017		https://doi.org/10.1103/PhysRevB.95.155203	No	Yes	Yes		Yes		3.836
24	*Excitonic effects in third-harmonic generation: The case of carbon nanotubes and nanoribbons* C. Attaccalite, E. Cannuccia, and M. Grüning Phys. Rev. B 95, 125403 (2017)	C. Attaccalite	3	C. Attaccalite, E. Cannuccia, and M. Grüning (UK)	WG2	25-07-2016		https://doi.org/10.1103/PhysRevB.95.125403	No	Yes	Yes		Yes		3.836
25	Unraveling the spin structure of unoccupied states in Bi2Se3 C. Datzer, A. Zumbulte, J. Braun, T. Forster, A. B. Schmidt, J. L. Mi, B. Iversen, P. Hofmann, J. Minar, H. Ebert, P. Kruger, M. Rohlfing, M. Donath Phys. Rev. B **95**, 115401 (2017)	C. Datzer	13	C. Datzer, A. Zumbulte, J. Braun (DE), T. Forster, A. B. Schmidt, J. L. Mi, B. Iversen, P. Hofmann, J. Minar (DE, MC Member, WG1 Leader), H. Ebert (DE, Chair), P. Kruger (JP, NNC Representative), M. Rohlfing, M. Donath	WG1 WG2 WG3 WG4	17-11-2016		https://doi.org/10.1103/PhysRevB.95.115401	No	Yes	Yes		Yes		3.836
26	*Anomalous anisotropic exciton temperature dependence in rutile TiO2* E. Baldini, A. Dominguez, L. Chiodo, E. Sheveleva, M. Yazdi-Rizi, C. Bernhard, A. Rubio, M. Chergui Phys. Rev. B 96, 041204 (2017)	E. Baldini	8	E. Baldini, A. Dominguez, L. Chiodo, E. Sheveleva, M. Yazdi-Rizi, C. Bernhard, A. Rubio (ES, MC	WG1 WG2 WG3	03-04-2017		https://doi.org/10.1103/PhysRevB.96.041204	No	Yes	Yes		Yes		3.836

				Member), M. Chergui											
27	*Ab initio Modelling of Plasmons in Metal-semiconductor Bilayer Transition-metal Dichalcogenide Heterostructures* H. S. Sen, L. D. Xian, F. H. da Jornada, S. G. Louie, A. Rubio Isr. J. Chem. **57**, 540-546 (2017)	H. S. Sen	5	H. S. Sen, L. D. Xian, F. H. da Jornada, S. G. Louie, A. Rubio (ES, MC Member)	WG1 WG2 WG3	21-09-2016		https://doi.org/10.1002/ijch.201600122	No	Yes	Yes		Yes		2.455
28	*Strongly bound excitons in anatase TiO2 single crystals and nanoparticles* E. Baldini, L. Chiodo, A. Dominguez, M. Palummo, S. Moser, M. Yazdi-Rizi, G. Aubock, B. P. P. Mallett, H. Berger, A. Magrez, C. Bernhard, M. Grioni, A. Rubio, M. Chergui Nature Communications **8**, 13 (2017)	E. Baldini	14	E. Baldini, L. Chiodo, A. Dominguez, M. Palummo (IT), S. Moser, M. Yazdi-Rizi, G. Aubock, B. P. P. Mallett, H. Berger, A. Magrez, C. Bernhard, M. Grioni, A. Rubio (ES, MC Member), M. Chergui	WG1 WG2 WG3	03-10-2016		https://doi.org/10.1038/s41467-017-00016-6	No	Yes	Yes		Yes		12.124
29	*Cavity Born-Oppenheimer Approximation for Correlated Electron-Nuclear-Photon Systems* J. Flick, H. Appel, M. Ruggenthaler, A. Rubio J. Chem. Theory Comput. **13**, 1616-1625 (2017)	J. Flick	4	J. Flick, H. Appel, M. Ruggenthaler, A. Rubio (ES, MC Member)	WG1 WG2 WG3	19-11-2016		https://doi.org/10.1021/acs.jctc.6b01126	No	Yes	Yes		Yes		5.245
30	*Dispersion and damping of the interband pi plasmon in graphene grown on Cu(111) foils* A. Politano, I. Radovic, D. Borka, Z. L. Miskovic, H. K. Yu, D. Farias, G. Chiarello Carbon **114**, 70-76 (2017)	A. Politano	7	A. Politano (IT), I. Radovic (RS), D. Borka (RS, MC Member), Z. L. Miskovic, H. K. Yu, D. Farias, G. Chiarello	WG2	05-10-2016		https://doi.org/10.1016/j.carbon.2016.11.073	No	Yes	Yes		Yes		6.337
31	*Efficient and accurate modeling of electron photoemission in nanostructures with TDDFT* P. Wopperer, U. De Giovannini, A. Rubio Eur. Phys. J. B **90**, 51 (2017)	P. Wopperer	3	P. Wopperer, U. De Giovannini (ES), A. Rubio (ES, MC Member)	WG1 WG2 WG3	19-09-2016		https://doi.org/10.1140/epjb/e2017-70548-3	No	Yes	Yes		Yes		1.461
32	*Impact of the Electronic Band Structure in High-Harmonic Generation Spectra of Solids* N. Tancogne-Dejean, O. D. Mucke, F. X. Kartner, A. Rubio Phys. Rev. Lett. 118, 087403 (2017)	N. Tancogne Dejean	4	N. Tancogne-Dejean, O. D. Mucke, F. X. Kartner, A. Rubio (ES, MC Member)	WG1 WG2 WG3	29-09-2016		https://doi.org/10.1103/PhysRevLett.118.087403	No	Yes	Yes		Yes		8.462
33	*h-AlN-Mg(OH)(2) van derWaals bilayer heterostructure: Tuning the excitonic characteristics* C. Bacaksiz, A. Dominguez, A. Rubio, R. T. Senger, H. Sahin Phys. Rev. B 95, 075423 (2017)	C. Bacaksiz	5	C. Bacaksiz, A. Dominguez, A. Rubio (ES, MC Member), R. T. Senger, H. Sahin	WG1 WG2 WG3	14-10-2016		https://doi.org/10.1103/PhysRevB.95.075423	No	Yes	Yes		Yes		3.836
34	*Local environment effects in the magnetic properties and electronic*	S. A. Khan	5	S. A. Khan, J. Minar (DE, MC	WG1 WG2	17-10-2016		https://doi.org/10.1103/PhysRevB.95.014408							3.836

	structure of disordered FePt S. A. Khan, J. Minar, H. Ebert, P. Blaha, O. Šipr Physical Review B **95**, 14408 (2017)			Member, WG1 Leader), H. Ebert (DE, Chair), P. Blaha (AT), O. Šipr (CZ)	WG3 WG4										
35	*Decomposition behavior of platinum clusters supported on ceria and gamma-alumina in the presence of carbon monoxide* I. Z. Koleva, H. A. Aleksandrov, G. N. Vayssilov Catal. Sci. Technol. **7**, 734-742 (2017)	I. Z. Koleva	3	I. Z. Koleva, H. A. Aleksandrov (BG, MC Member), G. N. Vayssilov	WG1	11-12-2016		https://doi.org/10.1039/c6cy02586b	No	Yes	Yes		Yes		5.773
36	*Creating stable Floquet-Weyl semimetals by laser-driving of 3D Dirac materials* H. Hubener, M. A. Sentef, U. De Giovannini, A. F. Kemper, A. Rubio Nature Communications **8**, 13940 (2017)	H. Hubener	5	H. Hubener, M. A. Sentef, U. De Giovannini (ES), A. F. Kemper, A. Rubio (ES, MC Member)	WG1 WG2 WG3	15-04-2016		https://doi.org/10.1038/ncomms13940	No	Yes	Yes		Yes		12.124
37	*Pressure induced phase transition in correlated oxides and simple metals: Mott and charge-transfer insulators* A. Rubio IOP Conf. Series: Journal of Physics Conf. Series **950**, 032003 (2017)	A. Rubio	1	A. Rubio (ES, MC Member)	WG1 WG2 WG3			https://doi.org/10.1088/1742-6596/950/3/032003	No	Yes	Yes		Yes		
38	*Magneto-optical reflection spectroscopy on graphene/Co in the soft x-ray range* H.-Ch. Mertins, C. Jansing, M. Gilbert, M. Krivenkov, J. Sanchez-Barriga, A. Varykhalov, O. Rader, H. Wahab, H. Timmers, A. Gaupp, M. Tesch, A. Sokolov, D. Legut, P. M. Oppeneer IOP Conf. Series: Journal of Physics: Conf. Series **903**, 012025 (2017)	H.-Ch. Mertins	14	H.-Ch. Mertins, C. Jansing, M. Gilbert, M. Krivenkov, J. Sanchez-Barriga, A. Varykhalov, O. Rader, H. Wahab, H. Timmers, A. Gaupp, M. Tesch, A. Sokolov, D. Legut (CZ), P. M. Oppeneer (SE)	WG2 WG3			https://doi.org/10.1088/1742-6596/903/1/012025	No	Yes	Yes		Yes		
39	*Near-Edge X-ray Absorption Fine Structure within Multilevel Coupled Cluster Theory* R. H. Myhre, S. Coriani, H. Koch J. Chem. Theory Comput. **12**, 2633–2643 (2016)	R. H. Myhre	3	R. H. Myhre (NO), S. Coriani (DK)	WG1 WG2 WG3	26-02-2016		https://doi.org/10.1021/acs.jctc.6b00216	No	Yes	Yes		Yes		5.245
40	*Coupled Cluster Study of Photoionization and Photodetachment Cross Sections* B. N. C. Tenorio, M. A. C. Nascimento, S. Coriani, A. B. Rocha J. Chem. Theory Comput. **12**, 4440–4459 (2016)	B. N. C. Tenorio	4	B. N. C. Tenorio, M. A. C. Nascimento, S. Coriani (DK), A. B. Rocha	WG1 WG2 WG3	20-05-2016		https://doi.org/10.1021/acs.jctc.6b00524	No	Yes	Yes		Yes		5.245
41	*Two-Step Phase Transition in SnSe and the Origins of its High Power Factor from First Principles* A. Dewandre, O. Hellman, S. Bhattacharya, A. H. Romero, G. K. H. Madsen,	A. Dewandre	6	A. Dewandre, O. Hellman, S. Bhattacharya, A. H. Romero, G. K. H. Madsen,	WG1 WG2 WG3 WG4	05-01-2016		https://doi.org/10.1103/PhysRevLett.117.276601	No	Yes	Yes		Yes		8.462

	M. J. Verstraete Phys. Rev. Lett. **117**, 276601 (2016)			M. J. Verstraete (BE, MC Member)											
42	*Universal steps in quantum dynamics with time-dependent potential-energy surfaces: Beyond the Born-Oppenheimer picture* G. Albareda, A. Abedi, I. Tavernelli, A. Rubio Phys. Rev. A **94**, 062511 (2016)	G. Albareda	4	G. Albareda, A. Abedi, I. Tavernelli, A. Rubio (ES, MC Member)	WG1 WG2 WG3	29-01-2016		https://doi.org/10.1103/PhysRevA.94.062511	No	Yes	Yes		Yes		2.925
43	*Structural, electronic and adsorption properties of Rh(111)/Mo(110) bimetallic catalyst: A DFT study* K. Palotas, I. Bako, L. Bugyi Appl. Surf. Science **389**, 1094-1103 (2016)	K. Palotas	3	K. Palotas (SK, MC Member), L. Bugyi (HU)	WG1 WG2	26-04-2016		https://doi.org/10.1016/j.apsusc.2016.08.020	No	Yes	Yes		Yes		3.387
44	*Polyyne electronic and vibrational properties under environmental interactions* M. Wanko, S. Cahangirov, L. Shi, P. Rohringer, Z. J. Lapin, L. Novotny, P. Ayala, T. Pichler, A. Rubio Phys. Rev. B **94**, 195422 (2016)	M. Wanko	9	M. Wanko, S. Cahangirov, L. Shi, P. Rohringer, Z. J. Lapin, L. Novotny, P. Ayala, T. Pichler, A. Rubio (ES, MC Member)	WG1 WG2 WG3	05-04-2016		https://doi.org/10.1103/PhysRevB.94.195422	No	Yes	Yes		Yes		3.836
45	*Negative plasmon dispersion in 2H-NbS2 beyond the charge-density-wave interpretation* P. Cudazzo, E. Muller, C. Habenicht, M. Gatti, H. Berger, M. Knupfer, A. Rubio, S. Huotari New Journal of Physics **18**, 103050 (2016)	P. Cudazzo	8	P. Cudazzo, A. Rubio (ES, MC Member)	WG1 WG2 WG3	28-05-2016		https://doi.org/10.1088/1367-2630/18/10/103050	No	Yes	Yes		Yes		3.786
46	*Nickel: The time-reversal symmetry conserving partner of iron on a chalcogenide topological insulator* M. Vondracek, L. Cornils, J. Minar, J. Warmuth, M. Michiardi, C. Piamonteze, L. Barreto, J. A. Miwa, M. Bianchi, Ph. Hofmann, L. Zhou, A. Kamlapure, A. A. Khajetoorians, R. Wiesendanger, J.-L. Mi, B.-B. Iversen, S. Mankovsky, S. Borek (DE), H. Ebert, M. Schuler, T. Wehling, J. Wiebe, J. Honolka Phys. Rev. B **94**, 161114 (2016)	M. Vondracek	23	M. Vondracek (CZ), J. Minar (DE, MC Member, WG1 Leader), S. Borek (DE), H. Ebert (DE, Chair)	WG1 WG2 WG3 WG4	07-04-2016		https://doi.org/10.1103/PhysRevB.94.161114	No	Yes	Yes		Yes		3.836
47	*Ab initio calculations of X-ray magnetic circular dichroism spectra within the projector augmented wave method: An implementation into the VASP code* A. Dixit, M. Alouani Computer Physics Communications **207**, 136-144 (2016)	A. Dixit	2	A. Dixit (FR), M. Alouani (FR)	WG1 WG2 WG3	08-03-2016		https://doi.org/10.1016/j.cpc.2016.05.022	No	Yes	Yes		Yes		3.936
48	*Disentangling Vacancy Oxidation on Metallicity-Sorted Carbon Nanotubes* D. J. Mowbray, A. P. Paz, G. Ruiz-Soria, M. Sauer, P. Lacovig, M. Dalmiglio, S. Lizzit, K. Yanagi, A. Goldoni, T. Pichler, P. Ayala, A. Rubio	D. J. Mowbray	12	D. J. Mowbray, A. Rubio (ES, MC Member)	WG1 WG2 WG3	17-07-2016		https://doi.org/10.1021/acs.jpcc.6b06163	No	Yes	Yes		Yes		4.536

	J. Phys. Chem. C **120**, 18316-18322 (2016)														
49	*Stability of the Dirac cone in artificial graphene formed in quantum wells: a computational many-electron study* I. Kylanpaa, F. Berardi, E. Rasanen, P. Garcia-Gonzalez, C. A. Rozzi, A. Rubio New Journal of Physics **18**, 083014 (2016)	I. Kylanpaa	6	I. Kylanpaa, A. Rubio (ES, MC Member)	WG1 WG2 WG3	20-06-2016		https://doi.org/10.1088/1367-2630/18/8/083014	No	Yes	Yes		Yes		3.786
50	*Quantum plasmonics: from jellium models to ab initio calculations* A. Varas, P. Garcia-Gonzalez, J. Feist, F. J. Garcia-Vidal, A. Rubio Nanophotonics **5**, 409-426 (2016)	A. Varas	5	A. Varas, P. Garcia-Gonzalez, J. Feist, F. J. Garcia-Vidal, A. Rubio (ES, MC Member)	WG1 WG2 WG3	12-11-2015		http://dx.doi.org/10.1515/nanoph-2015-0141	No	Yes	Yes		Yes		3.114
51	*New Graphical User Interface for EXAFS analysis with the GNXAS suite of programs* K. Hatada, F. Iesari, L. Properzi, M. Minicucci and A. di Cicco J. Phys.: Conf. Ser. **712**, 012002 (2016).	K. Hatada	5	K. Hatada (FR) F. Iesari (IT) A. di Cicco (IT)	WG2 WG4 WG5			http://stacks.iop.org/1742-6596/712/i=1/a=012002	No	Yes	Yes		Yes		
52	*Recent developments in the ABINIT software package* X. Gonze, F. Jollet, F. A. Araujo, D. Adams, B Amadon, T. Applencourt, C. Audouze, J.-M. Beuken, J. Bieder, A. Bokhanchuk, E. Bousquet, F. Bruneval, D. Caliste, M. Cote, F. Dahm, F. Da Pieve, M. Delaveau, M. Di Gennaro, B. Dorado, C. Espejo, G. Geneste, L. Genovese, A. Gerossier, M. Giantomassi, Y. Gillet, D. R. Hamann, L. He, G. Jomard, J. L. Janssen, S. Le Roux, A. Levitt, A. Lherbier, F. Liu, I. Lukacevic, A. Martin, C. Martins, M. J. T. Oliveira, S. Ponce, Y. Pouillon, T. Rangel, G.-M. Rignanese, A. H. Romero, B. Rousseau, O. Rubel, A. A. Shukri, M. Stankovski, M. Torrent, M. J. Van Setten, B. Van Troeye, M. J. Verstraete, D. Waroquiers, J. Wiktor, B. Xu, A. Zhou, J. W. Zwanziger Computer Physics Communications 205, 106-131 (2016)	X. Gonze	55	X. Gonze, Y. Pouillon (ES), T. Rangel, G.-M. Rignanese (BE, MC Member, WG1 Deputy Leader), M. J. Verstraete (BE, MC Member),	WG1 WG2 WG3 WG4	14-01-2016		https://doi.org/10.1016/j.cpc.2016.04.003	No	Yes	Yes		Yes		3.936
53	*Exact maps in density functional theory for lattice models* T. Dimitrov, H. Appel, J. I. Fuks, A. Rubio New Journal of Physics **18**, 083004 (2016)	T. Dimitrov	4	T. Dimitrov, H. Appel, J. I. Fuks, A. Rubio (ES, MC Member)	WG1 WG2 WG3	23-03-2016		https://doi.org/10.1088/1367-2630/18/8/083004	No	Yes	Yes		Yes		3.786
54	*Electronic Structure of Low-Dimensional Carbon pi-Systems* c, I. Boukahil, R. M. Qiao, A. Rubio, F. J. Himpsel J. Phys. Chem. C **120**, 12362-12368 (2016)	J. M. Garcia-Lastra	5	J. M. Garcia-Lastra, A. Rubio (ES, MC Member), F. J. Himpsel	WG1 WG2 WG3	10-03-2016		https://doi.org/10.1021/acs.jpcc.6b02530	No	Yes	Yes		Yes		4.536
55	*Confined linear carbon chains as a route to bulk carbyne* L. Shi, P. Rohringer, K. Suenaga, Y. Niimi, J.	L. Shi	14	L. Shi, P. A. Rubio (ES, MC Member), Y. J.	WG1 WG2 WG3	25-09-2014		https://doi.org/10.1038/NMAT4617	No	Yes	Yes		Yes		39.737

	Kotakoski, J. C. Meyer, H. Peterlik, M. Wanko, S. Cahangirov, A. Rubio, Y. J. Lapin, L. Novotny, P. Ayala, T. Pichler Nature Materials **15**, 634 (2016)			Lapin, L. Novotny, P. Ayala, T. Pichler											
56	*ES2MS: An interface package for passing self-consistent charge density and potential from Electronic Structure codes To Multiple Scattering codes* J. Q. Xu, C. R. Natoli, P. Kruger, K. Hayakawa, D. Sebilleau, L. Song, K. Hatada Comp. Phys. Commun. **203**, Pages: 331-338 (2016)	J. Q. Xu	7	C. R. Natoli (IT), P. Kruger (JP, NNC Representative), D. Sebilleau (FR, Vice Chair), K. Hatada (FR)	WG1 WG2 WG3 WG4	04-10-2015		https://doi.org/10.1016/j.cpc.2016.02.031	No	Yes	Yes		Yes		3.936
57	*Tailored pump-probe transient spectroscopy with time-dependent density-functional theory: controlling absorption spectra* J. Walkenhorst, U. De Giovannini, A. Castro, A. Rubio Eur. Phys. J. B **89**, 128 (2016)	J. Walkenhorst	5	J. Walkenhorst, U. De Giovannini (ES), A. Castro, A. Rubio (DE, MC Member)	WG1 WG2 WG3	22-01-2016		https://doi.org/10.1140/epjb/e2016-70064-0	No	Yes	Yes		Yes		1.461
58	*On the Exciton Coupling between Two Chlorophyll Pigments in the Absence of a Protein Environment: Intrinsic Effects Revealed by Theory and Experiment* B. F. Milne, C. Kjaer, J. Houmoller, M. H. Stockett, Y. Toker, A. Rubio, S. B. Nielsen Angew. Chem. Int. Ed. **55**, 6248-6251 (2016)	B. F. Milne	7	A. Rubio (ES, MC Member), S. B. Nielsen (DK)	WG1 WG2 WG3	25-02-2016		https://doi.org/10.1002/anie.201601979	No	Yes	Yes		Yes		11.994
59	*Theoretical Insight into the Internal Quantum Efficiencies of Polymer/C-60 and Polymer/SWNT Photovoltaic Devices* L. N. Glanzmann, D. J. Mowbray J. Phys. Chem. C **120**, 6336-6343 (2016)	L. N. Glanzmann	2	L. N. Glanzmann, D. J. Mowbray		24-12-2015		https://doi.org/10.1021/acs.jpcc.5b12611	No	Yes	Yes		Yes		4.536
60	*On the possibility of using X-ray Compton scattering to study magnetoelectrical properties of crystals* S. P. Collins, D. Laundy, T. Connolley, G. van der Laan, F. Fabrizi, O. Janssen, M. J. Cooper, H. Ebert, S. Mankovsky Acta Cryst. A **72**, 197-205 (2016)	S. P. Collins	9	S. P. Collins, G. van der Laan (UK, MC Member, ARS Contact), H. Ebert (DE, Chair)	WG1 WG2 WG3 WG4	16-10-2015		https://doi.org/10.1107/S2053273316000863	No	Yes	Yes		Yes		5.725
61	*Density functional theory study of the alpha-gamma phase transition in cerium: Role of electron correlation and f-orbital localization* M. Casadei, X. G. Ren, P. Rinke, A. Rubio, M. Scheffler Phys. Rev. B 93, 075153 (2016)	M. Casadei	5	M. Casadei, X. G. Ren, P. Rinke, A. Rubio (ES, MC Member), M. Scheffler	WG1 WG2 WG3	22-07-2015		https://doi.org/10.1103/PhysRevB.93.075153	No	Yes	Yes		Yes		3.836
62	*Anisotropic electronic, mechanical, and optical properties of monolayer WTe2* E. Torun, H. Sahin, S. Cahangirov, A. Rubio, F. M. Peeters J. Appl. Phys. **119**, 074307 (2016)	E. Torun	5	E. Torun, H. Sahin, S. Cahangirov, A. Rubio (ES, MC Member), F. M.	WG1 WG2 WG3	04-11-2015		https://doi.org/10.1063/1.4942162	No	Yes	Yes		Yes		2.068

				Peeters											
63	*Ultrafast reflectivity dynamics of highly excited Si surfaces below the melting transition* R. Gunnella, G. Zgrablic, E. Giangrisostomi, F. D'Amico, E. Principi, C. Masciovecchio, A. Di Cicco and F. Parmigiani Phys. Rev. B **94**, 155427 (2016).	R. Gunnella	8	R. Gunnella (IT, MC Member, WG3 Leader) A. Di Cicco (IT) F. Parmigiani (DE)	WG3 WG5	29-10-2015		http://link.aps.org/doi/10.1103/PhysRevB.94.155427	No	Yes	Yes		Yes		3.836
64	*Fermi Surface Manipulation by External Magnetic Field Demonstrated for a Prototypical Ferromagnet* E. Mlynczak, M. Eschbach, S. Borek (DE), J. Minar, J. Braun (DE), I. Aguilera, G. Bihlmayer, S. Doring, M. Gehlmann, P. Gospodaric, S. Suga, L. Plucinski, S. Blugel, H. Ebert, C. M. Schneider Phys. Rev. X 6, 041048 (2016)	E. Mlynczak	15	S. Borek (DE), J. Minar (DE, MC Member, WG1 Leader), J. Braun (DE), H. Ebert (DE, Chair), E. Mlynczak (PL)	WG1 WG2 WG3 WG4	01-05-2016		https://doi.org/10.1103/PhysRevX.6.041048	No	Yes	Yes		Yes		12.789
65	*Determination of surface and interface magnetic properties for the multiferroic heterostructure Co/BaTiO3 using spleed and arpes* S. Borek, J. Braun, J. Minar, D. Kutnyakhov, H. J. Elmers, G. Schonhense, H. Ebert J. Phys. Cond. Matter 28, 436004 (2016)	S. Borek	7	S. Borek (DE), J. Braun (DE), J. Minar (DE, MC Member, WG1 Leader), H. Ebert (DE, Chair)	WG1 WG2 WG3 WG4	01-07-2016		https://doi.org/10.1088/0953-8984/28/43/436004	No	Yes	Yes		Yes		2.649
66	*One-step theory of two-photon photoemission* J. Braun, R. Rausch, M. Potthoff, H. Ebert Phys. Rev. B 94, 125128 (2016)	J. Braun	4	J. Braun (DE), H. Ebert (DE, Chair)	WG1 WG2 WG3 WG4	23-07-2016		https://doi.org/10.1103/PhysRevB.94.125128	No	Yes	Yes		Yes		3.836
67	*Local electron-electron interaction strength in ferromagnetic nickel determined by spin-polarized positron annihilation* H. Ceeh, J. A. Weber, P. Boni, M. Leitner, D. Benea, L. Chioncel, H. Ebert, J. Minar, D. Vollhardt, C. Hugenschmidt Scientific Reports **6**, 20898 (2016)	H. Ceeh	10	D. Benea (RO, MC Member), H. Ebert (DE, Chair), J. Minar (DE, MC Member, WG1 Leader)	WG1 WG2 WG3 WG4	13-10-2015		https://doi.org/10.1038/srep20898	No	Yes	Yes		Yes		4.259
68	*High Pressure Vibrational Properties of WS2 Nanotubes* K. R. O'Neal, J. G. Cherian, A. Zak, R. Tenne, Z. Liu, J. L. Musfeldt Nano Lett. **16**, 993-999 (2016)	K. R. O'Neal	6	K. R. O'Neal, J. G. Cherian, A. Zak (IL, MC Member), R. Tenne, Z. Liu, J. L. Musfeldt	WG5	01-10-2015		https://doi.org/10.1021/acs.nanolett.5b03996	No	Yes	Yes		Yes		12.712
69	*Dynamics of Photoelectrons and Structural Changes of Tungsten Trioxide Observed by Femtosecond Transient XAFS* Y. Uemura, D. Kido, Y. Wakisaka, H. Uehara, T. Ohba, Y. Niwa, S. Nozawa, T. Sato, K. Ichiyanagi, R. Fukaya, S. Adachi, T. Katayama, T. Togashi, S. Owada, K. Ogawa, M. Yabashi, K. Hatada, S. Takakusagi, T.	Y. Uemura	21	K. Hatada (FR), S. Takakusagi, T. Yokoyama, B. Ohtani, K. Asakura	WG1 WG2 WG3 WG4	03-10-2015		https://doi.org/10.1002/anie.201509252	No	Yes	Yes		Yes		11.994

	Yokoyama, B. Ohtani, K. Asakura Agew. Chem. Int. Ed. **55**, 1364-1367 (2016)														
70	*Fully relativistic multiple scattering theory for general potentials* H. Ebert, J. Braun, D. Kodderitzsch, and S. Mankovsky Phys. Rev. B **93**, 075145 (2016)	H. Ebert	4	H. Ebert (DE, Chair), J. Braun (DE), D. Kodderitzsch, S. Mankovsky	WG1 WG2 WG3 WG4	11-12-2015		https://doi.org/10.1103/PhysRevB.93.075145							
71	*Spilling of electronic states in Pb quantum wells* M. Jalochowski, K. Palotas, M. Krawiec Phys. Rev. B **93**, 035437 (2016)	M. Jalochowski	3	M. Jalochowski, K. Palotas (HU, MC Member), M. Krawiec	WG1 WG2	02-08-2015		https://doi.org/10.1103/PhysRevB.93.035437	No	Yes	Yes		Yes		3.836
72	*The mechanical bond on carbon nanotubes: diameter-selective functionalization and effects on physical properties* E. Martinez-Perinan, A. de Juan, Y. Pouillon, C. Schierl, V. Strauss, N. Martin, A. Rubio, D. M. Guldi, E. Lorenzo, E. M. Perez Nanoscale **8**, 9254-9264 (2016)	E. Martinez-Perinan	10	E. Martinez-Perinan, Y. Pouillon (ES), A. Rubio (ES, MC Member)	WG1 WG2 WG3	10-02-2016		https://doi.org/10.1039/c6nr01182a	No	Yes	Yes		Yes		7.367
73	*Interband plasmons in supported graphene on metal substrates: Theory and experiments* A. Politano, I. Radovic, D. Borka, Z. L. Miskovic, G. Chiarello CARBON **96**, 91-97 (2016)	A. Politano	5	A. Politano (IT), I. Radovic (RS), D. Borka (RS, MC Member)	WG2	31-07-2015		https://doi.org/10.1016/j.carbon.2015.09.053	No	Yes	Yes		Yes		6.337
74	*Radiation damage on Langmuir monolayers of the anionic 1.2-dipalmitoyl-sn-glycero-3-[phospho-rac-(1-glycerol)] (sodium salt) (DPPG) phospholipid at the air-DNA solution interface* P. J. Gomes, A. M. P. S. G. da Silva, P. A. Ribeiro, O. N. Jr. Oliveira, M. Raposo MATERIALS SCIENCE & ENGINEERING C-MATERIALS FOR BIOLOGICAL APPLICATIONS **58**, 576-579 (2016)	P. J. Gomes	5	P. J. Gomes, A. M. P. S. G. da Silva, P. A. Ribeiro, O. N. Jr. Oliveira, M. Raposo (PT, MC Member)	WG2	03-03-2015		https://doi.org/10.1016/j.msec.2015.09.017	No	Yes	Yes		Yes		4.164
75	*Communication: X-ray absorption spectra and core-ionization potentials within a core-valence separated coupled cluster framework* S. Coriani, H. Koch J. Chem. Phys. **143**, 181103 (2015)	S. Coriani	2	S. Coriani (DK), H. Koch (NO)	WG1 WG2 WG3	20-09-2015		https://doi.org/10.1063/1.4935712	No	Yes	Yes		Yes		2.965
76	*Kohn-Sham approach to quantum electrodynamical density-functional theory: Exact time-dependent effective potentials in real space* J. Flick, M. Ruggenthaler, H. Appel, A. Rubio PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA **112**, 15285-15290 (2-15)	J. Flick	4	J. Flick, M. Ruggenthaler, H. Appel, A. Rubio (ES, MC Member)	WG1 WG2 WG3	14-09-2015		https://doi.org/10.1073/pnas.1518224112	No	Yes	Yes		Yes		9.661

77	*Multiferroic heterostructures for spin filter applications: An ab initio study* S. Borek (DE), J. Braun (DE), H. Ebert, J. Minar Phys. Rev. B 92, 174408 (2015)	S. Borek	4	S. Borek (DE), J. Braun (DE), H. Ebert (DE, Chair), J. Minar (DE, MC Member, WG1 Leader)	WG1 WG2 WG3 WG4	13-10-2015		https://doi.org/10.1103/PhysRevB.92.174408	No	Yes	Yes		Yes		3.836
78	*Ab initio calculation of spin-polarized low-energy electron diffraction pattern for the systems Fe(001) and Fe(001)- p(1x1)O* S. Borek (DE), J. Braun (DE), J. Minar, H. Ebert Phys. Rev. B 92, 075126 (2015)	S. Borek	4	S. Borek (DE), J. Braun (DE), J. Minar (DE, MC Member, WG1 Leader), H. Ebert (DE, Chair)	WG1 WG2 WG3 WG4	24-07-2015		https://doi.org/10.1103/PhysRevB.92.075126	No	Yes	Yes		Yes		3.836
79	*Anomalous d-like surface resonances on Mo(110) analyzed by time-of-flight momentum microscopy* S. V. Chernov, K. Medjanik, C. Tusche, D. Kutnyakhov, S. A. Nepijko, A. Oelsner, J. Braun (DE), J. Minar, S. Borek (DE), H. Ebert, H. J. Elmers, J. Kirschner, G. Schonhense Ultramicroscopy, **159** Special Issue: SI, 453-463 (2015)	S. V. Chernov	13	S. V. Chernov, J. Braun (DE), J. Minar (DE, MC Member, WG1 Leader), S. Borek (DE), H. Ebert (DE, Chair)	WG1 WG2 WG3 WG4	14-11-2014		https://doi.org/10.1016/j.ultramic.2015.07.008	No	Yes	Yes		Yes		2.843
80	*X-ray absorption spectra of graphene and graphene oxide by full-potential multiple scattering calculations with self-consistent charge density* J.Q. Xu, P. Kruger, C. R. Natoli, K. Hayakawa, Z. Y. Wu, K. Hatada Phys. Rev. B **92**, 125408 (2015)	J.Q. Xu	6	J.Q. Xu, P. Kruger (JP, NNC Representative), C. R. Natoli (IT), K. Hatada (FR)	WG1 WG2 WG3 WG4	10-06-2015		https://doi.org/10.1103/PhysRevB.92.125408	No	Yes	Yes		Yes		3.836
81	*Orbitals from local RDMFT: Are they Kohn-Sham or natural orbitals?* I. Theophilou, N. N. Lathiotakis, N. I. Gidopoulos, A. Rubio, N. Helbig J. Chem. Phys. **143**, 054106 (2015)	I. Theophilou	5	I. Theophilou, N. N. Lathiotakis (GR, MC Member), A. Rubio (ES, MC Member)	WG1 WG2 WG3	04-05-2015		https://aip.scitation.org/doi/pdf/10.1063/1.4927784	No	Yes	Yes		Yes		2.965
82	*Enhancing and controlling single-atom high-harmonic generation spectra: a time-dependent density-functional scheme* A. Castro, A. Rubio, E. K. U. Gross Eur. Phys. J. B 88 : 191 (2015)	A. Castro	3	A. Castro (ES), A. Rubio (ES, MC Member), E. K. U. Gross	WG1 WG2 WG3	30-12-2014		https://link.springer.com/content/pdf/10.1140%2Fepjb%2Fe2015-50889-7.pdf	No	Yes	Yes		Yes		1.461
83	*Comparing Quasiparticle H2O Level Alignment on Anatase and Rutile TiO2* H. Sun, D. J. Mowbray, A. Migani, J. Zhao, H. Petek, A. Rubio ACS Catal. 5 (7), pp 4242–4254 (2015)	H. Sun	6	H. Sun, D. J. Mowbray, A. Migani, J. Zhao, H. Petek, A. Rubio (ES, MC Member)	WG1 WG2 WG3	12-03-2015		https://pubs.acs.org/doi/pdf/10.1021/acscatal.5b00529	No	Yes	Yes		Yes		10.614
84	*Fermi Surface of Three-Dimensional La1-xSrxMnO3 Explored by Soft-X-Ray ARPES:*	L. L. Lev	15	L. L. Lev, J. P. Blaha (AT, MC	WG1 WG2	11-11-2014		https://doi.org/10.1103/PhysRevLett.114.237601	No	Yes	Yes		Yes		8.462

	Rhombohedral Lattice Distortion and its Effect on Magnetoresistance L. L. Lev, J. Krempasky, U. Staub, V. A. Rogalev, T. Schmitt, M. Shi, P. Blaha, A. S. Mishchenko, A. A. Veligzhanin, Y. V. Zubavichus, M. B. Tsetlin, H. Volfova, J. Braun (DE), J. Minar, V. N. Strocov Phys. Rev. Lett. **114**, 237601 (2015)			Member), J. Braun (DE), J. Minar (DE, MC Member, WG1 Leader)	WG3										
85	*Momentum-Resolved Spin Dynamics of Bulk and Surface Excited States in the Topological Insulator Bi2Se3* C. Cacho, A. Crepaldi, M. Battiato, J. Braun, F. Cilento, M. Zacchigna, M. C. Richter, O. Heckmann, E. Springate, Y. Liu, S. S. Dhesi, H. Berger, Ph. Bugnon, K. Held, M. Grioni, H. Ebert, K. Hricovini, J. Minar, and F. Parmigiani Phys. Rev. Lett. **114**, 097401 (2015)	C. Cacho	19	C. Cacho, J. Braun (DE), H. Ebert (DE, Chair), K. Hricovini, J. Minar (DE, MC Member, WG1 Leader)	WG1 WG2 WG3 WG4	15-09-2014		https://doi.org/10.1103/PhysRevLett.114.097401	No	Yes	Yes		Yes		8.462
86	*Large Seebeck effect by charge-mobility engineering* P. J. Sun, B. P. Wei, J. H. Zhang, J. M. Tomczak, A. M. Strydom, M. Sondergaard, B. B. Iversen, F. Steglich Nature Communications, **6**, 7475 (2015)	P. J. Sun	8	P. J. Sun, J. H. Zhang, J. M. Tomczak (AT)	WG2	18-03-2015		https://www.nature.com/articles/ncomms8475	No	Yes	Yes		Yes		12.124
87	*Conditional Born-Oppenheimer Dynamics: Quantum Dynamics Simulations for the Model Porphine* G. Abareda, J. M. Bofill, I. Tavernelli, F. Huarte-Larranaga, F. Illas, A. Rubio J. Phys. Chem. Lett. **6**, 1529-1535 (2015)	G. Abareda	6	G. Abareda, F. Huarte-Larranaga, A. Rubio (ES, MC Member)		27-02-2015		https://pubs.acs.org/doi/abs/10.1021/acs.jpclett.5b00422	No	Yes	Yes		Yes		9.353
88	*Exciton dispersion in molecular solids* P. Cudazzo, F. Sottile, A. Rubio, M. Gatti J. Phys.: Condens. Matter **27**, 113204 (2015)	P. Cudazzo	4	P. Cudazzo, F. Sottile, A. Rubio (ES, MC Member), M. Gatti		30-09-2014		https://doi.org/10.1088/0953-8984/27/11/113204	No	Yes	Yes		Yes		2.649
89	*Modifying the Interlayer Interaction in Layered Materials with an Intense IR Laser* Y. Miyamoto, H. Zhang, T. Miyazaki, A. Rubio Phys. Rev. Lett. **114**, 116102 (2015)	Y. Miyamoto	4	Y. Miyamoto, H. Zhang, T. Miyazaki, A. Rubio (ES, MC Member)		12-01-2015		https://doi.org/10.1103/PhysRevLett.114.116102	No	Yes	Yes		Yes		8.462
90	*Real-space grids and the Octopus code as tools for the development of new simulation approaches for electronic systems* X. Andrade, D. Strubbe, U. De Giovannini, A. H. Larsen, M. J. T. Oliveira, J. Alberdi-Rodriguez, A. Varas, I. Theophilou, N. Helbig, M. J. Verstraete, L. Stella, F. Nogueira, A. Aspuru-Guzik, A. Castro, M. A. L.	X. Andrade	16	X. Andrade, U. De Giovannini (ES), M. J. T. Oliveira (BE), Verstraete (BE, MC Member), F. Nogueira (PT), A. Castro (ES),	WG1 WG2 WG3	19-01-2015		https://doi.org/10.1039/c5cp00351b	No	Yes	Yes		Yes		4.123

	Marques, A. Rubio Phys. Chem. Chem. Phys. 17, 31371-31396 (2015)			A. Rubio (ES, MC Member)											
91	Optical field terahertz amplitude modulation by graphene nanoribbons H. Zhang, Y. Miyamoto, X. L. Cheng, A. Rubio Nanoscale **7**, 19012-19017 (2015)	H. Zhang	4	H. Zhang, Y. Miyamoto, X. L. Cheng, A. Rubio (ES, MC Member)	WG2	28-08-2015		https://doi.org/10.1039/c5nr05889a	No	Yes	Yes		Yes		7.367
92	*Insights into colour-tuning of chlorophyll optical response in green plants* J. Jornet-Somoza, J. Alberdi-Rodriguez, B. F. Milne, X. Andrade, M. A. L. Marques, F. Nogueira, M. J. T. Oliveira, J. J. P. Stewart, A. Rubio Phys. Chem. Chem. Phys., **17**, 26599-26606 (2015)	J. Jornet-Somoza	9	J. Jornet-Somoza (ES), M. A. L. Marques (DE), F. Nogueira (PT), M. J. T. Oliveira (BE), A. Rubio (ES, MC Member)		11-06-2015		https://doi.org/10.1039/c5cp03392f	No	Yes	Yes		Yes		4.123
93	*The Soret absorption band of isolated chlorophyll a and b tagged with quaternary ammonium ions* M. H. Stockett, L. Musbat, C. Kjaer, J. Houmoller, Y. Toker, A. Rubio, B. F. Milne, S. B. Nielsen Phys. Chem. Chem. Phys., **17**, 25793-25798 (2015)	M. H. Stockett	8	M. H. Stockett (DK), L. Musbat (IL), C. Kjaer (DK), J. Houmoller, Y. Toker, A. Rubio (ES, MC Member)		15-07-2016		https://doi.org/10.1039/c5cp01513h	Yes	Yes	Yes		Yes		4.123
94	*Exploring the optoelectronic structure and thermoelectricity of recent photoconductive chalcogenides compounds, CsCdInQ(3) (Q = Se, Te)* W. Khan, S. Goumri-Said RSC ADVANCES 5, 9455-9461 (2015)	W. Khan	2	W. Khan (CZ), S. Goumri-Said		29-10-2014		https://doi.org/10.1039/c4ra13426e	No	Yes	Yes		Yes		3.108
95	*Interplay of electron heating and saturable absorption in ultrafast extreme ultraviolet transmission of condensed matter* A. Di Cicco, K. Hatada, E. Giangrisostomi, R. Gunnella, F Bencivenga, E. Principi, C. Masciovecchio, A. Filipponi Phys. Rev. B 90, 220303 (2014)	A. Di Cicco	8	A. Di Cicco (IT), K. Hatada (FR), R. Gunnella (IT, MC Member, WG3 Leader)		08-09-2014		https://doi.org/10.1103/PhysRevB.90.220303	No	Yes	Yes		Yes		3.836
96	*Quantum electrodynamical time-dependent density-functional theory for many-electron systems on a lattice* M. Farzanehpour, I. V. Tokatly Phys. Rev. B 90, 195149 (2014)	M. Farzanehpour,	2	M. Farzanehpour (ES), I. V. Tokatly (ES)		27-08-2014		https://doi.org/10.1103/PhysRevB.90.195149	Yes	Yes	Yes		Yes		3.836
97	*Ab initio nanoplasmonics: The impact of atomic structure* P. Zhang, J. Feist, A. Rubio, P. Garcia-	P. Zhang	5	P. Zhang, J. Feist, A. Rubio (ES, MC		14-02-2014		https://doi.org/10.1103/PhysRevB.90.161407	No	Yes	Yes		Yes		3.836

	Gonzalez, F. J. Garcia-Vidal Phys. Rev. B 90, 161407 (2014)			Member), P. Garcia-Gonzalez, F. J. Garcia-Vidal											
98	*Induced work function changes at Mg-doped MgO/Ag(001) interfaces: Combined Auger electron diffraction and density functional study* T. Jaouen, P. Aebi, S. Tricot, G. Delhaye, B. Lepine, D. Sebilleau, G. Jezequel, P. Schieffer Phys. Rev. B 90, 125433 (2014)	T. Jaouen	8	T. Jaouen (CH), P. Aebi (CH), S. Tricot (FR), G. Delhaye (FR), B. Lepine (FR), D. Sebilleau (FR, Vice Chair), G. Jezequel (FR), P. Schieffer (FR)	WG4	10-07-2014		https://doi.org/10.1103/PhysRevB.90.125433	No	Yes	Yes		Yes		3.836