Yves Ferro

List of Publications by Year
in descending order

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50 papers	1,631 citations	304368 22 h-index	301761 39 g-index
50 all docs	50 docs citations	50 times ranked	1658 citing authors

#	Article	IF	Citations
1	Hydrogen diffusion and vacancies formation in tungsten: Density Functional Theory calculations and statistical models. Acta Materialia, 2015, 94, 307-318.	3.8	174
2	Density functional theory investigation of the diffusion and recombination of H on a graphite surface. Chemical Physics Letters, 2003, 368, 609-615.	1.2	122
3	Density functional theory investigation of H adsorption and H2 recombination on the basal plane and in the bulk of graphite: Connection between slab and cluster model. Journal of Chemical Physics, 2002, 116, 8124-8131.	1.2	120
4	Dissociative adsorption of small molecules at vacancies on the graphite (0001) surface. Carbon, 2006, 44, 3320-3327.	5.4	107
5	Stability and magnetism of hydrogen dimers on graphene. Physical Review B, 2008, 78, .	1.1	103
6	Plasmaâ€“wall interaction studies within the EUROfusion consortium: progress on plasma-facing components development and qualification. Nuclear Fusion, 2017, 57, 116041.	1.6	75
7	Adsorption, diffusion, and recombination of hydrogen on pure and boron-doped graphite surfaces. Journal of Chemical Physics, 2004, 120, 11882-11888.	1.2	58
8	Hydrogen adsorption on graphite (0001) surface: A combined spectroscopyâ€“density-functional-theory study. Journal of Chemical Physics, 2005, 123, 124701.	1.2	55
9	Experimental and Theoretical UV Characterizations of Acetylacetone and Its Isomers. Journal of Physical Chemistry A, 2006, 110, 3920-3926.	1.1	51
10	Density functional theory investigation of H adsorption on the basal plane of boron-doped graphite. Journal of Chemical Physics, 2003, 118, 5650-5657.	1.2	49
11	Adsorption of NH3 on MgO(100): a comparative study of ab initio and semi-classical calculations. Surface Science, 1995, 325, 139-150.	0.8	48
12	Quantum study of hydrogenâ€“oxygenâ€“graphite interactions. Carbon, 2004, 42, 3189-3198.	5.4	44
13	Saturation of tungsten surfaces with hydrogen: A density functional theory study complemented by low energy ion scattering and direct recoil spectroscopy data. Acta Materialia, 2018, 145, 388-398.	3.8	36
14	Sodium hydroxide formation in water clusters: The role of hydrated electrons and the influence of electric field. Journal of Chemical Physics, 2003, 118, 10461-10469.	1.2	30
15	Hydrogenation and dehydrogenation of graphite (0001) surface: a density functional theory study. Physica Scripta, 2006, T124, 91-95.	1.2	30
16	Theoretical study of oxygen adsorption on boron-doped graphite. Surface Science, 2004, 559, 158-168.	0.8	28
17	Electron solvation by highly polar molecules: Density functional theory study of atomic sodium interaction with water, ammonia, and methanol. Journal of Chemical Physics, 2004, 120, 8683-8691.	1.2	27
18	Study of hydrogen isotopes behavior in tungsten by a multi trapping macroscopic rate equation model. Physica Scripta, 2016, T167, 014011.	1.2	27

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19	Reaction-diffusion modeling of hydrogen transport and surface effects in application to single-crystalline Be. Nuclear Instruments & Methods in Physics Research B, 2018, 430, 23-30.	0.6	27
20	Self-assembled molecular chains formed by selective adsorption of leadâ€“phthalocyanine on InSb(100)-(4Ã—2)/c(8Ã—2). Applied Physics Letters, 2003, 82, 2518-2520.	1.5	26
21	Surface coverage dependent mechanisms for the absorption and desorption of hydrogen from the W(1â€‰1â€‰0) and W(1â€‰0â€‰0) surfaces: a density functional theory investigation. Nuclear Fusion, 2019, 59, 106022.	1.6	25
22	Model for thermal desorption of hydrogen atoms from a graphite surface based on kinetic Monte Carlo simulations. Physical Review B, 2008, 77, .	1.1	22
23	Hydrogen supersaturated layers in H/D plasma-loaded tungsten: A global model based on thermodynamics, kinetics and density functional theory data. Physical Review Materials, 2018, 2, .	0.9	22
24	UV and IR photoisomerizations of an intramolecularly H-bonded molecule: acetylacetone trapped in nitrogen matrix. Chemical Physics Letters, 2003, 370, 118-125.	1.2	21
25	Interpretation of STM images of graphite with an atomic vacancy via density-functional calculations of electronic structure. Physical Review B, 2007, 75, .	1.1	21
26	First-Principles Study of hydrogen retention and diffusion in beryllium oxide. Solid State Ionics, 2015, 272, 91-100.	1.3	20
27	Identification of BeO and BeOxDy in melted zones of the JET Be limiter tiles: Raman study using comparison with laboratory samples. Nuclear Materials and Energy, 2018, 17, 295-301.	0.6	20
28	Absorption and diffusion of beryllium in graphite, beryllium carbide formation investigated by density functional theory. Journal of Applied Physics, 2013, 113, 213514.	1.1	16
29	Electronic transitions and resonance electron scattering measured by electron energy loss spectroscopy of lead phthalocyanine thin film. Thin Solid Films, 2004, 466, 259-264.	0.8	15
30	Hydrogen retention in beryllium: concentration effect and nanocrystalline growth. Journal of Physics Condensed Matter, 2015, 27, 475401.	0.7	15
31	Analytical bond order potential for simulations of BeO 1D and 2D nanostructures and plasma-surface interactions. Journal of Physics Condensed Matter, 2018, 30, 135001.	0.7	15
32	Density functional study of chemical erosion mechanisms in carbon and boron-doped carbon as plasma facing material in tokamaks. Journal of Nuclear Materials, 2003, 321, 294-304.	1.3	14
33	Evidence of hydrogenated hexamers on graphite. Chemical Physics Letters, 2009, 478, 42-44.	1.2	14
34	Theoretical investigation on the point defect formation energies in beryllium and comparison with experiments. Nuclear Materials and Energy, 2017, 12, 453-457.	0.6	14
35	Adsorption of beryllium atoms and clusters both on graphene and in a bilayer of graphite investigated by DFT. Journal of Physics Condensed Matter, 2013, 25, 015002.	0.7	13
36	Electron solvation by polar molecules:â€‚The interaction of Na atoms with solid methanol films studied with MIES and density functional theory calculations. Journal of Chemical Physics, 2004, 120, 8692-8697.	1.2	12

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37	Modelling tritium adsorption and desorption from tungsten dust particles with a surface kinetic model. Nuclear Fusion, 2021, 61, 086030.	1.6	12
38	The interaction of beryllium with benzene and graphene: a comparative investigation based on DFT, MP2, CCSD(T), CAS-SCF and CAS-PT2. Physical Chemistry Chemical Physics, 2014, 16, 1957-1966.	1.3	11
39	Hydrogen retention and diffusion in tungsten beryllide. Journal of Physics Condensed Matter, 2014, 26, 315012.	0.7	11
40	Diffusivity of hydrogen and properties of point defects in beryllium investigated by DFT. Journal of Nuclear Materials, 2019, 524, 323-329.	1.3	11
41	Kinetic model for hydrogen absorption in tungsten with coverage dependent surface mechanisms. Nuclear Fusion, 2020, 60, 106011.	1.6	11
42	Isotopic effects in the sticking of H and D atoms on the (0 0 0 1) graphite surface. Chemical Physics Letters, 2009, 477, 225-229.	1.2	10
43	Preparing the future post-mortem analysis of beryllium-based JET and ITER samples by multi-wavelengths Raman spectroscopy on implanted Be, and co-deposited Be. Nuclear Fusion, 2017, 57, 076035.	1.6	10
44	Modelling of hydrogen isotopes trapping, diffusion and permeation in divertor monoblocks under ITER-like conditions. Nuclear Fusion, 2021, 61, 126003.	1.6	9
45	Hydrogen in beryllium oxide investigated by DFT: on the relative stability of charged-state atomic versus molecular hydrogen. Journal of Physics Condensed Matter, 2018, 30, 305201.	0.7	8
46	Predictive Atomistic Model for Hydrogen Adsorption on Metal Surfaces: Comparison with Low-Energy Ion Beam Analysis on Tungsten. Journal of Physical Chemistry C, 2021, 125, 16086-16096.	1.5	8
47	A density functional theory based thermodynamic model of hydrogen coverage on the W(110) surface. Physica Scripta, 2020, T171, 014025.	1.2	6
48	Contribution to a better evaluation of the dust speciation in case of an accident in ITER. Fusion Engineering and Design, 2017, 124, 1171-1176.	1.0	4
49	Electron delocalization by polar molecules: Interaction of Na atoms with solid ammonia films studied with MIES and density functional theory. Journal of Chemical Physics, 2004, 121, 3717-3721.	1.2	2
50	D retention and material defects probed using Raman microscopy in JET limiter samples and beryllium-based synthesized samples. Physica Scripta, 2021, 96, 124031.	1.2	2