

# Pu00e4r At Olsson

## List of Publications by Year in descending order

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Version: 2024-02-01

32  
papers

897  
citations

567281

15  
h-index

454955

30  
g-index

32  
all docs

32  
docs citations

32  
times ranked

918  
citing authors

#	ARTICLE	IF	CITATIONS
1	Ab initio study of Cr interactions with point defects in bcc Fe. Physical Review B, 2007, 75, .	3.2	269
2	Ab initio thermodynamics of zirconium hydrides and deuterides. Computational Materials Science, 2014, 86, 211-222.	3.0	64
3	Semi-empirical atomistic study of point defect properties in BCC transition metals. Computational Materials Science, 2009, 47, 135-145.	3.0	61
4	On the importance of surface elastic contributions to the flexural rigidity of nanowires. Journal of the Mechanics and Physics of Solids, 2012, 60, 2064-2083.	4.8	50
5	Atomistic simulations of tensile and bending properties of single-crystal bcc iron nanobeams. Physical Review B, 2007, 76, .	3.2	41
6	Transverse resonant properties of strained gold nanowires. Journal of Applied Physics, 2010, 108, .	2.5	37
7	All-atomic and coarse-grained molecular dynamics investigation of deformation in semi-crystalline lamellar polyethylene. Polymer, 2018, 153, 305-316.	3.8	35
8	High temperature nanoindentation hardness and Young's modulus measurement in a neutron-irradiated fuel cladding material. Journal of Nuclear Materials, 2017, 487, 113-120.	2.7	30
9	First principles characterisation of brittle transgranular fracture of titanium hydrides. Acta Materialia, 2016, 118, 362-373.	7.9	29
10	Atomistic study of the buckling of gold nanowires. Acta Materialia, 2011, 59, 3883-3894.	7.9	26
11	On the role of hydrogen filled vacancies on the embrittlement of zirconium: An ab initio investigation. Journal of Nuclear Materials, 2015, 467, 311-319.	2.7	26
12	Ab initio thermodynamics investigation of titanium hydrides. Computational Materials Science, 2015, 97, 263-275.	3.0	25
13	Investigation of microstructure evolution during self-annealing in thin Cu films by combining mesoscale level set and ab initio modeling. Journal of the Mechanics and Physics of Solids, 2016, 90, 160-178.	4.8	24
14	The Influence of shearing and rotary inertia on the resonant properties of gold nanowires. Journal of Applied Physics, 2010, 108, 104312.	2.5	21
15	Ab initio and classical atomistic modelling of structure and defects in crystalline orthorhombic polyethylene: Twin boundaries, slip interfaces, and nature of barriers. Polymer, 2017, 121, 234-246.	3.8	19
16	Effects of interatomic potential on fracture behaviour in single- and bicrystalline tungsten. Computational Materials Science, 2022, 207, 111283.	3.0	16
17	First principles investigation of the finite temperature dependence of the elastic constants of zirconium, magnesium and gold. Computational Materials Science, 2015, 99, 361-372.	3.0	15
18	Ab initio investigation of monoclinic phase stability and martensitic transformation in crystalline polyethylene. Physical Review Materials, 2018, 2, .	2.4	14

#	ARTICLE	IF	CITATIONS
19	Intergranular fracture of tungsten containing phosphorus impurities: A first principles investigation. Computational Materials Science, 2017, 139, 368-378.	3.0	12
20	Relation between thermal expansion and interstitial formation energy in pure Fe and Cr. Nuclear Instruments & Methods in Physics Research B, 2005, 228, 122-125.	1.4	11
21	Inverse structural modification using constraints. Journal of Sound and Vibration, 2007, 303, 767-779.	3.9	10
22	Ab initio-based fracture toughness estimates and transgranular traction-separation modelling of zirconium hydrides. Modelling and Simulation in Materials Science and Engineering, 2015, 23, 045015.	2.0	10
23	Structure of two-dimensional Fe3O4. Journal of Chemical Physics, 2020, 152, 114705.	3.0	10
24	Structural Changes in Monolayer Cobalt Oxides under Ambient Pressure CO and O <sub>2</sub> Studied by In Situ Grazing-Incidence X-ray Absorption Fine Structure Spectroscopy. Journal of Physical Chemistry C, 2022, 126, 3411-3418.	3.1	9
25	On the natural vibrations of linear structures with constraints. Journal of Sound and Vibration, 2007, 301, 341-354.	3.9	6
26	Experimental and numerical assessment of the work of fracture in injection-moulded low-density polyethylene. Engineering Fracture Mechanics, 2018, 192, 1-11.	4.3	6
27	Theoretical and Experimental Aspects of Current and Future Research on NbO2 Thin Film Devices. Crystals, 2021, 11, 217.	2.2	6
28	Atomistic investigation of functionalized polyethylene-alumina interfacial strength and tensile behaviour. Computational Materials Science, 2021, 187, 110075.	3.0	5
29	Hard and soft materials: putting consistent van der Waals density functionals to work. Electronic Structure, 2022, 4, 014001.	2.8	4
30	Stability, magnetic order, and electronic properties of ultrathin $\text{FeO}_4$ nanosheets. Physical Review B, 2020, 101, .	3.2	3
31	Atomistic Studies of the Elastic Properties of Metallic BCC Nanowires and Films. IUTAM Symposium on Cellular, Molecular and Tissue Mechanics, 2009, , 221-230.	0.2	3
32	Ab initio modelling of intergranular fracture of nickel containing phosphorus: Interfacial excess properties. Nuclear Materials and Energy, 2021, 28, 101055.	1.3	0