

# Pu00e4r At Olsson

## List of Publications by Year in descending order

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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	Hard and soft materials: putting consistent van der Waals density functionals to work. <i>Electronic Structure</i> , 2022, 4, 014001.	2.8	4
2	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. <i>Journal of Physical Chemistry C</i> , 2022, 126, 3411-3418.	3.1	9
3	Effects of interatomic potential on fracture behaviour in single- and bicrystalline tungsten. <i>Computational Materials Science</i> , 2022, 207, 111283.	3.0	16
4	Atomistic investigation of functionalized polyethylene-alumina interfacial strength and tensile behaviour. <i>Computational Materials Science</i> , 2021, 187, 110075.	3.0	5
5	Theoretical and Experimental Aspects of Current and Future Research on NbO <sub>2</sub> Thin Film Devices. <i>Crystals</i> , 2021, 11, 217.	2.2	6
6	Ab initio modelling of intergranular fracture of nickel containing phosphorus: Interfacial excess properties. <i>Nuclear Materials and Energy</i> , 2021, 28, 101055.	1.3	0
7	Structure of two-dimensional Fe <sub>3</sub> O <sub>4</sub> . <i>Journal of Chemical Physics</i> , 2020, 152, 114705.	3.0	10
8	Stability, magnetic order, and electronic properties of ultrathin Fe <sub>3</sub> O <sub>4</sub> nanosheets. <i>Physical Review B</i> , 2020, 101, .	3.2	3
9	Experimental and numerical assessment of the work of fracture in injection-moulded low-density polyethylene. <i>Engineering Fracture Mechanics</i> , 2018, 192, 1-11.	4.3	6
10	All-atomic and coarse-grained molecular dynamics investigation of deformation in semi-crystalline lamellar polyethylene. <i>Polymer</i> , 2018, 153, 305-316.	3.8	35
11	Ab initio investigation of monoclinic phase stability and martensitic transformation in crystalline polyethylene. <i>Physical Review Materials</i> , 2018, 2, .	2.4	14
12	High temperature nanoindentation hardness and Young's modulus measurement in a neutron-irradiated fuel cladding material. <i>Journal of Nuclear Materials</i> , 2017, 487, 113-120.	2.7	30
13	Ab initio and classical atomistic modelling of structure and defects in crystalline orthorhombic polyethylene: Twin boundaries, slip interfaces, and nature of barriers. <i>Polymer</i> , 2017, 121, 234-246.	3.8	19
14	Intergranular fracture of tungsten containing phosphorus impurities: A first principles investigation. <i>Computational Materials Science</i> , 2017, 139, 368-378.	3.0	12
15	First principles characterisation of brittle transgranular fracture of titanium hydrides. <i>Acta Materialia</i> , 2016, 118, 362-373.	7.9	29
16	Investigation of microstructure evolution during self-annealing in thin Cu films by combining mesoscale level set and ab initio modeling. <i>Journal of the Mechanics and Physics of Solids</i> , 2016, 90, 160-178.	4.8	24
17	Ab initio-based fracture toughness estimates and transgranular traction-separation modelling of zirconium hydrides. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2015, 23, 045015.	2.0	10
18	First principles investigation of the finite temperature dependence of the elastic constants of zirconium, magnesium and gold. <i>Computational Materials Science</i> , 2015, 99, 361-372.	3.0	15

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19	Ab initio thermodynamics investigation of titanium hydrides. Computational Materials Science, 2015, 97, 263-275.	3.0	25
20	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
21	Ab initio thermodynamics of zirconium hydrides and deuterides. Computational Materials Science, 2014, 86, 211-222.	3.0	64
22	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
23	Atomistic study of the buckling of gold nanowires. Acta Materialia, 2011, 59, 3883-3894.	7.9	26
24	Transverse resonant properties of strained gold nanowires. Journal of Applied Physics, 2010, 108, .	2.5	37
25	The Influence of shearing and rotary inertia on the resonant properties of gold nanowires. Journal of Applied Physics, 2010, 108, 104312.	2.5	21
26	Semi-empirical atomistic study of point defect properties in BCC transition metals. Computational Materials Science, 2009, 47, 135-145.	3.0	61
27	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
28	Atomistic simulations of tensile and bending properties of single-crystal bcc iron nanobeams. Physical Review B, 2007, 76, .	3.2	41
29	Ab initio study of Cr interactions with point defects in bcc Fe. Physical Review B, 2007, 75, .	3.2	269
30	On the natural vibrations of linear structures with constraints. Journal of Sound and Vibration, 2007, 301, 341-354.	3.9	6
31	Inverse structural modification using constraints. Journal of Sound and Vibration, 2007, 303, 767-779.	3.9	10
32	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