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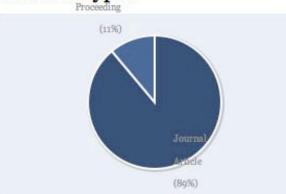
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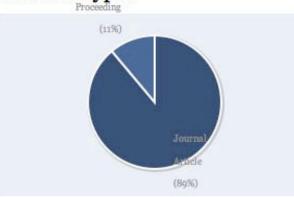
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Ab initio study of the composition dependence of the pressure-induced spin crossover in perovskite (Mg1-x,Fex)SiO3

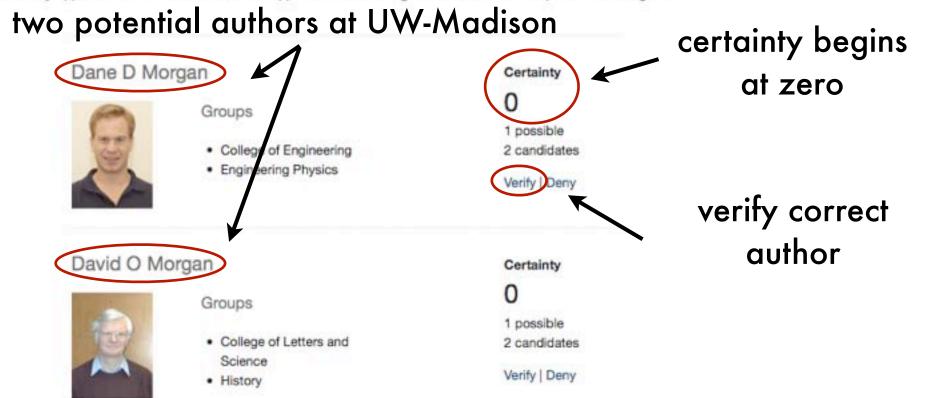
NameStrings: Bengtson, A.1 Persson, K Morgan, D.

Source: Earth and Planetary Science Letters 265(3-4), 535-45.

Year: 2008



ab initio calculations density functional theory Earth mantle geochemistry high-pressure effects iron compounds magnesium compounds minerals ab initio calculation perovskite Earth lower mantle composition dependence iron spin transition pressure iron concentration ferropericlase iron structural environment Local Density Approximation Generalized Gradient Approximation exchange-correlation methods spin crossover MgFeSiO3



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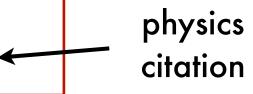
ADMIN::Contributions

Ab initio study of oxygen-vacancy ordering in oxygen conducting Ba2In2O5

NameStrings: Yueh-Lin Lee' Morgan, D.1

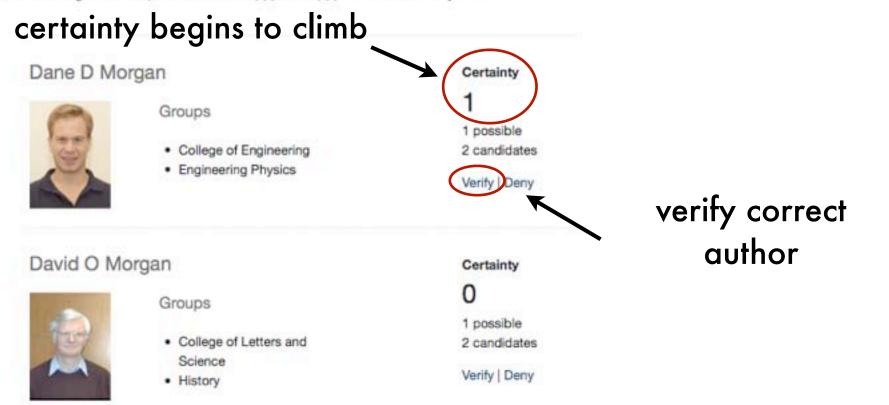
Source: Unknown (), 71-6.

Year: 2006



Keywords

ab initio calculations barium compounds Monte Carlo methods order-disorder transformations thermodynamic properties vacancies (crystal) ab initio simulation oxygen-vacancy ordering oxygen conducting Ba2ln2O5 Monte Carlo simulation cluster expansion first-order orthorhombic-tetragonal phase transition second-order tetragonal-cubic phase transition O(3) plane O(2) plane Ba2ln2O5 - System



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High-throughput and data mining with ab initio methods

NameStrings Morgan, D.) Ceder, G.1 Curtarolo, S.

Source: Measurement Science & Technology 16(1), 296-301.

Year: 2005



ab initio calculations chemistry computing computational complexity data mining physics computing very large databases ab initio methods high-throughput computation robust methods computational screening crystal structure prediction iterative algorithm computational speed large databases

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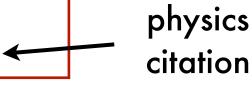
Thermodynamics of spinel LixTiO2 from first principles

NameStrings: Wagemaker, M.1 Van Der Ven, A. Morgan, D. Ceder, G. Mulder, F.M. Kearley, G.J.

Publishers

Source: Chemical Physics 317(2-3), 130-6.

Year: 2005



Keywords

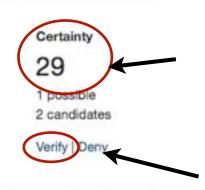
Generalized Gradient Approximation Monte Carlo methods thermodynamic properties Monte Carlo simulation cluster expansion Crystal structure chemical potential electrochemical electrodes ground states lithium compounds pseudopotential methods secondary cells solid solutions LixTiO2 spinel thermodynamics first principles study structural properties cluster expansion method pseudopotential ground state energy calculations GGA configurational thermodynamics Li configuration insertion potential Li composition two-phase region crystallographic site occupation unit cell dimension change X-ray diffraction experiment neutron diffraction experiment LixTiO2 solid solution behavior Li extraction potential step calculation Co spinel Mn-spinel electrode material battery material 300 K LixTiO2

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NameStrings: Morgan, D.

Source: Tis-the Times Literary Supplement (5427), 33-33.

Year: 2007



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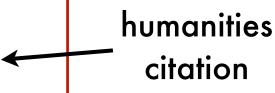
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· Eurasian transformations, tenth to thirteenth centuries: Crystallizations, divergences, renaissances.

NameStrings: Morgan, D.

Source: Speculum-J.Mediev.Stud. 82(1), 158-159.

Year: 2007



Keywords

Medieval & Renaissance Studies

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 NameStrings: Morgan, D.

Source: Tis-the Times Literary Supplement (5324), 15-15.

Year: 2005

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· Tameriane: Sword of Islam, conqueror of the world

NameStrings: Morgan, D.

Source: Tis-the Times Literary Supplement (5313), 6-7.

Year: 2005



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