Electronic-Structure-Based Design of Ordered Alloys

We describe some recent advances in the methodology of using electronic structure calculations for materials design. The methods have been developed for the design of ordered metallic alloys and metal alloy catalysts, but the considerations we present are relevant for the atomic-scale computational design of other materials as well. A central problem is how to treat the huge number of compounds that can be envisioned by varying the concentrations and the number of the elements involved. We discuss various strategies for approaching this problem and show how one strategy has led to the computational discovery of a promising catalytic metal alloy surface with high reactivity and low cost.

General information
State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Pages: 986-990
Publication date: 2006
Peer-reviewed: Yes

Publication information
Journal: M R S Bulletin
Volume: 31
Issue number: 12
ISSN (Print): 0883-7694
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.19 SJR 1.974 SNIP 1.559
Web of Science (2017): Impact factor 4.788
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.2 SJR 2.197 SNIP 1.613
Web of Science (2016): Impact factor 5.199
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 4.68 SJR 2.6 SNIP 2.143
Web of Science (2015): Impact factor 6.06
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 3.61 SJR 2.048 SNIP 1.943
Web of Science (2014): Impact factor 5.667
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 3 SJR 2 SNIP 1.581
Web of Science (2013): Impact factor 5.069
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 3.04 SJR 2.12 SNIP 1.917
Web of Science (2012): Impact factor 5.024
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 3.29 SJR 2.138 SNIP 1.921
Web of Science (2011): Impact factor 4.95
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.535 SNIP 2.164
Web of Science (2010): Impact factor 4.764
BFI (2009): BFI-level 1