ISA-TAB-Nano-Expanded: Community-Sourced Updated Templates

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NanoWG

Nancy Birkner, Ph.D.
Postdoctoral Associate
Center for the Environmental Implications of NanoTechnology
Pratt School of Engineering
Duke University
Durham, NC 27708

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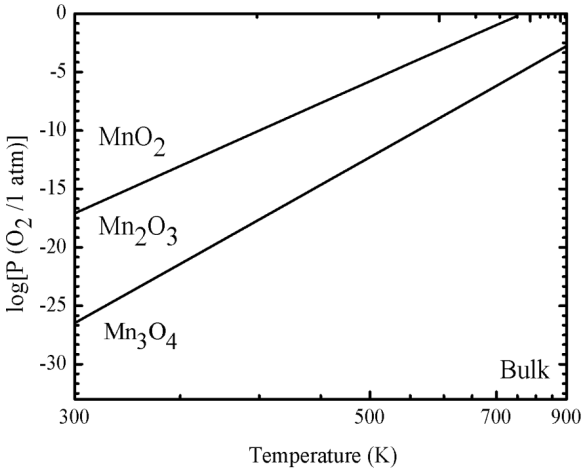
Issue: Nanophase transition metal oxides show large thermodynamically driven shifts in oxidation–reduction equilibria

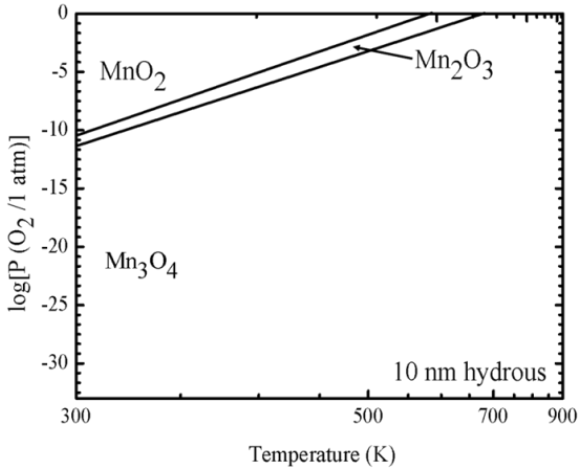
- Spinels, M_3O_4, have lower surface energies than divalent oxides MO and trivalent oxides M_2O_3, which expands the spinel stability field.
- At the nanoscale, dramatic Gibbs free-energy shifts occur for metal oxides that are not expected of coarse particles based on bulk-scale thermodynamics
- These trends may be a general phenomena of all metal oxide systems

  Navrotsky A, Ma C, Lilova K, Birkner N (2010) Science.

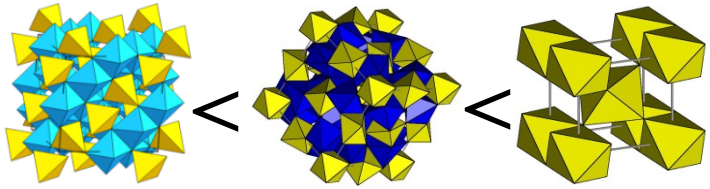
  Birkner and Navrotsky (2012).

UCDAVIS PETER A. ROCK Thermochemistry Laboratory





Surface Energy (SE) trend:

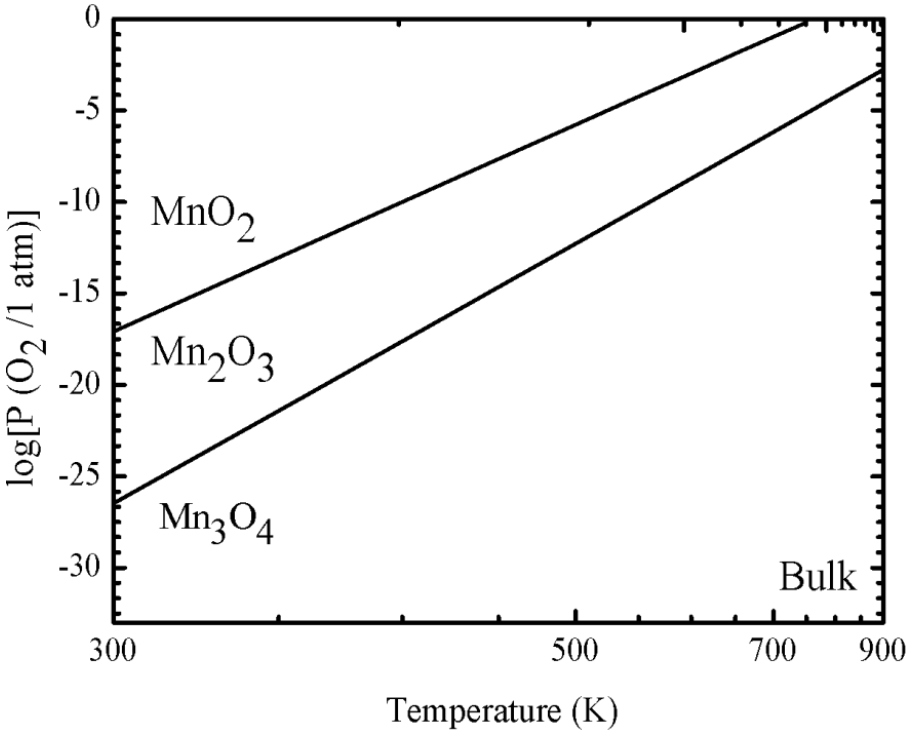


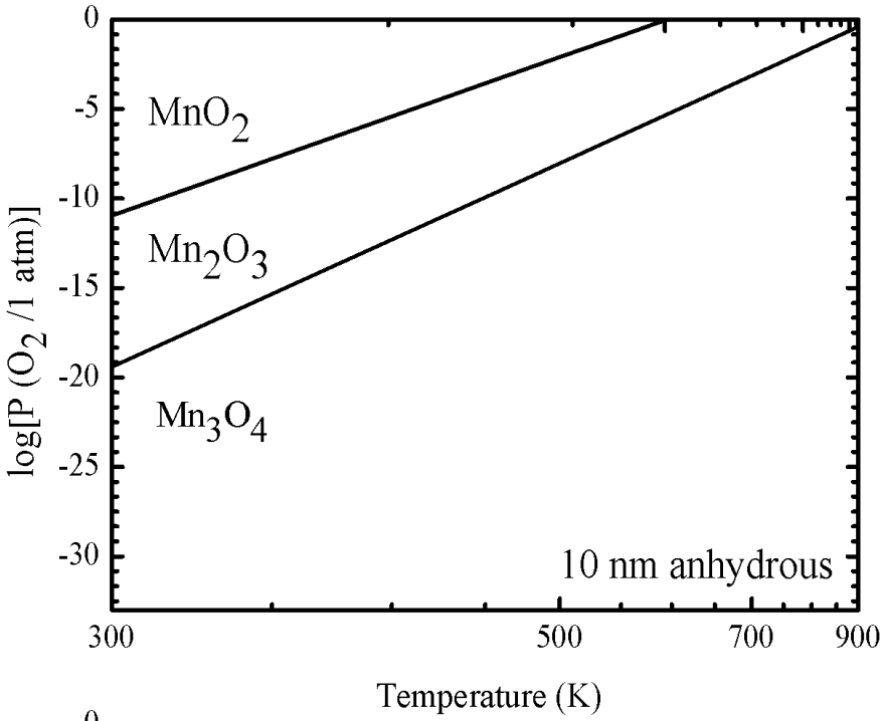
Mn_3O_4 < Mn_2O_3 < MnO_2

SE: hydrous < anhydrous

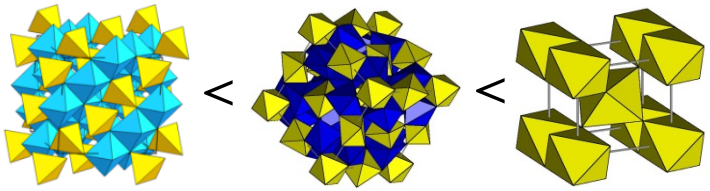
Surface free energy (SFE) shift favors the nanophase of lower surface energy.

Surface hydration enhances SFE shifts.

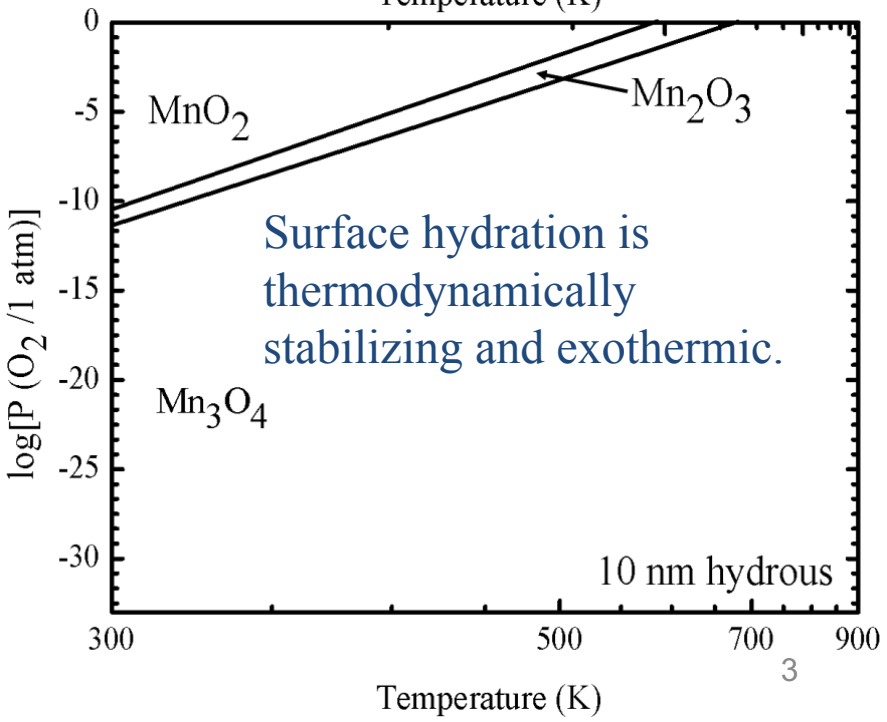




Surface Energy trend:



SE hydrous surface < anhydrous surface



Birkner and Navrotsky (2012)

Issue: What needed to be updated

Nanomaterial prior to experiment exposure, for example:

- Synthesis or purchased
- Mineral phase ID
- Nascent characteristics/behavior relevant to the assay (size, potential, surface chemistry, shape, crystal system…)
- Material state changes (dry to wet or wet to dry) of the nascent nanomaterial prior to experiment exposure

Experiment conditions to which the nanomaterial is exposed, for example:

- Media content
- Experiment conditions (T, stirring, columns, duration…)

Post-processing of exposed nanomaterial (if relevant), e.g.:

- Material state changes (dry to wet or wet to dry) of the nanomaterial after experiment exposure

Minimum parameters needed for a specific assay

Locations of ISA-TAB-Nano-Extended Templates

CEINT ISA-TAB-Nano-Extended webpage location:
https://ceint.duke.edu/research/nikc/isa-tab-nano

Functional Assay Templates
(Of note, these are the Alpha affinity and Dissolution templates)

Physical-Chemical Characterization Templates

in vivo Mammalian Toxicity Templates

in vitro Mammalian Toxicity Templates

Where are We Now & What's Next

- Suggested comment collection was completed
- Development of additional physical-chemical templates (Alpha and Dissolution) was completed.
- Data input into our Alpha and Dissolution templates was tested by collaborators
  - Minimum amount of experiment parameter input for each assay was found
  - Maximum amount depends upon the experiment design; templates may be further modified as needed by experimenters
- Nanomaterial instances are indicated in the experiment exposure section as this is where the variables are located
- It's time to hand off the baton to ASTM
- Beyond data collection…

NNKC

Image: http://pratt.duke.edu/about/news/setting-ground-rules-nanotechnology-research

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