PRISMS Center

Center for PRedictive Integrated Structural Materials Science

CASM Tutorial

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PRISMS Workshop 2021

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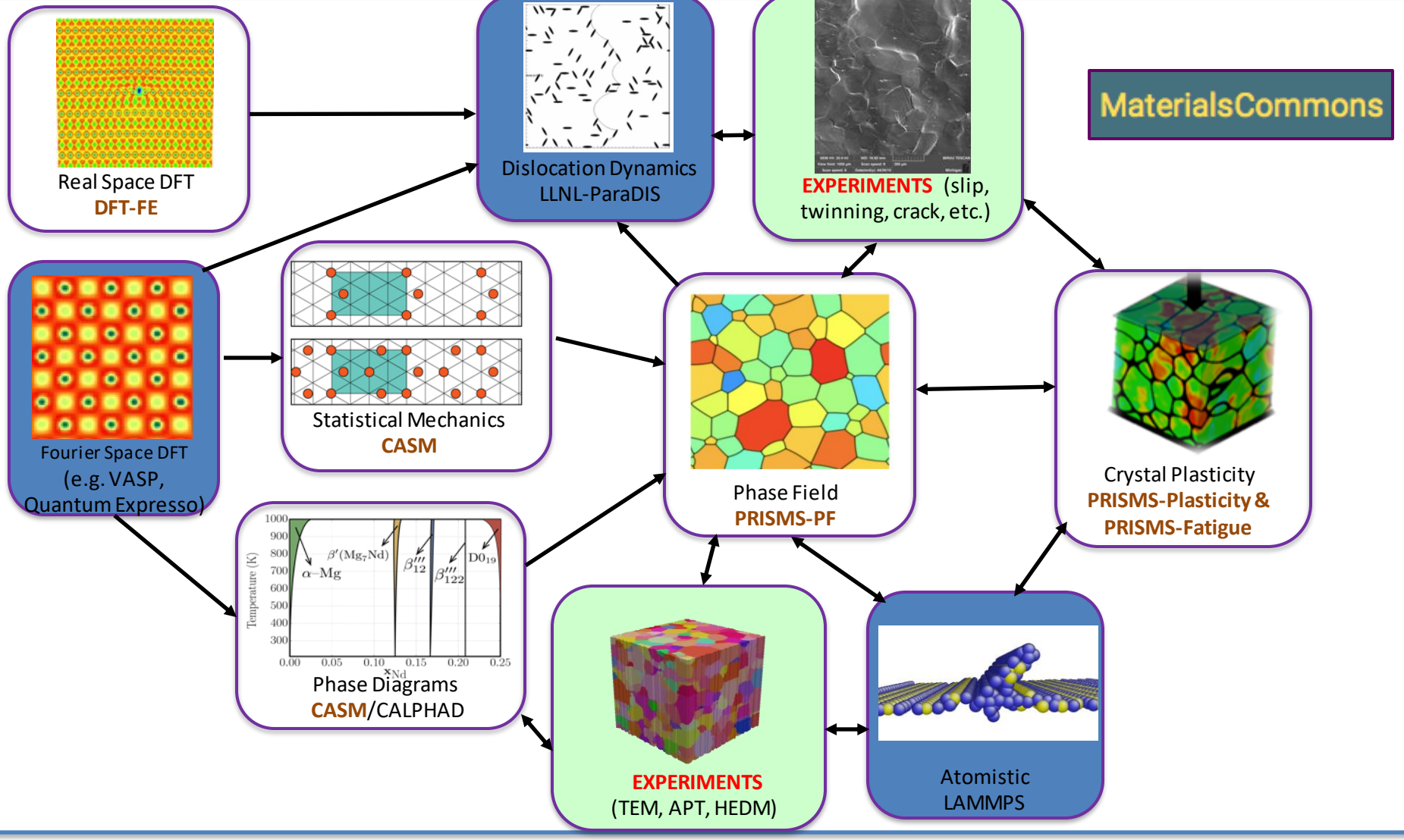
Center for PRedictive Integrated Structural Materials Science

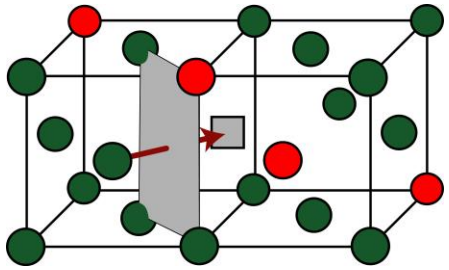
PRISMS

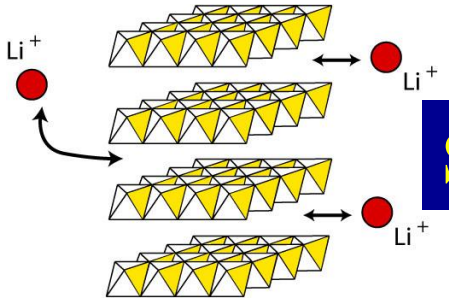
PRISMS Center Integrated Framework

Enabling accelerated predictive materials science



Electronic structure





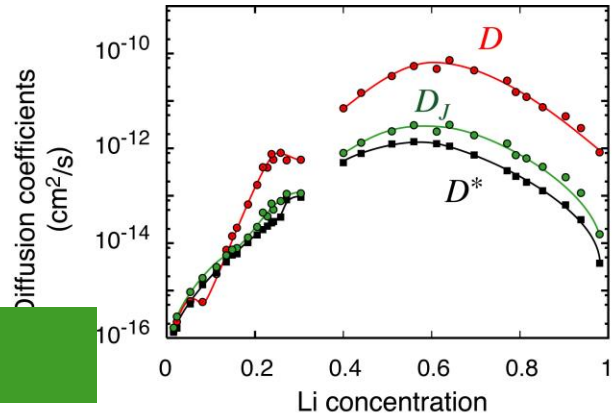
Statistical Mechanics

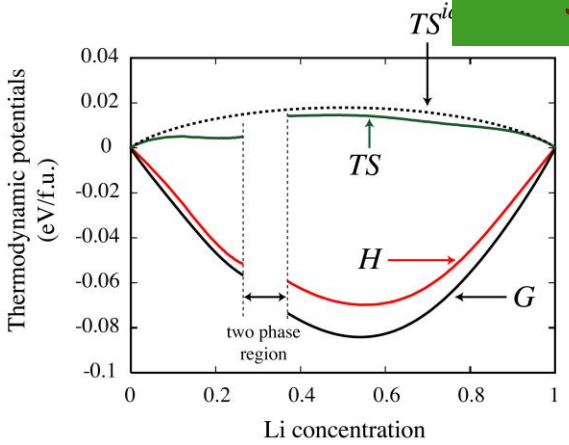
Linking atomistic descriptions to phenomenological models of materials

Thermodynamics

Kinetics

Solid Mechanics





Phenomenological descriptions

Electronic structure

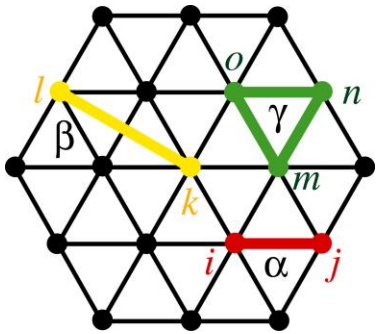
$$\left[-\nabla_i^2 + V_{ion}(r_i) + \int \frac{\rho(r')}{r-r'}dr' + V_{xc}(\rho(r_i))\right]\phi_i(r_i) = \varepsilon_i\phi(r_i)$$

Via rigorous and arbitrarily extendible cluster expansion Hamiltonians

Cluster Expansion Hamiltonians

$$E(\vec{\sigma}) = V_o + \sum_i V_i\sigma_i + \sum_{i,j} V_{i,j}\sigma_i\sigma_j + \sum_{i,j,k} V_{i,j,k}\sigma_i\sigma_j\sigma_k + \ldots$$

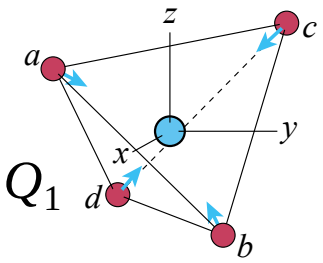
$$E(\vec{u}_1,..,\vec{u}_i,...,\vec{u}_N) = V_0 + \sum_{a,m} V_m^{(a)}F_m^{(a)}(\vec{Q}^{(a)}) + \sum_{b,n} V_n^{(b)}F_n^{(b)}(\vec{Q}^{(b)}) + \sum_{g,p} V_p^{(g)}F_p^{(g)}(\vec{Q}^{(g)}) + \ldots$$



Statistical Mechanics

$$F = -k_B T \ln Z$$

$$Z = \sum_s \exp\left(-\frac{E_s}{k_B T}\right)$$



Phenomenological descriptions

CASM Tutorial Outline

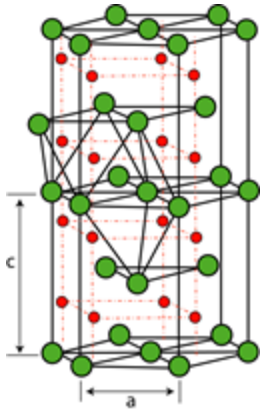
Day 1:

- Cluster expansion formulation
- Defining the "prim"
- Enumeration
- Occupation basis set construction

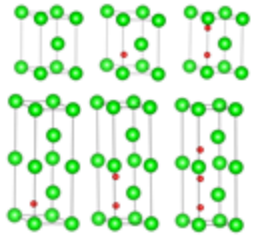
Day 2:

- DFT Calculation
- Parameterizing cluster expansions
- Monte Carlo
- Free energy integration and phase diagram construction

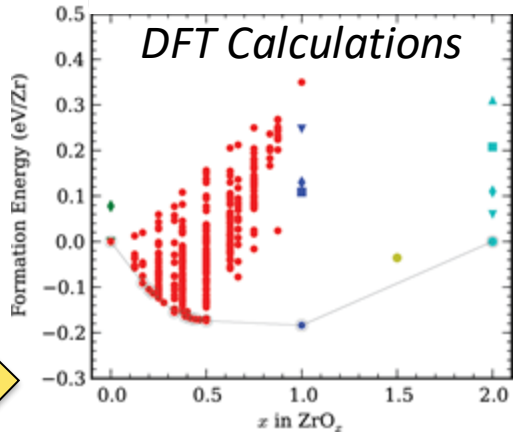
CASM Project Workflow

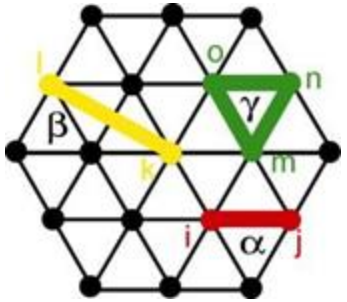


Primitive crystal structure



Enumerated configurations

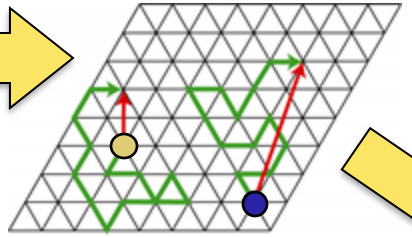




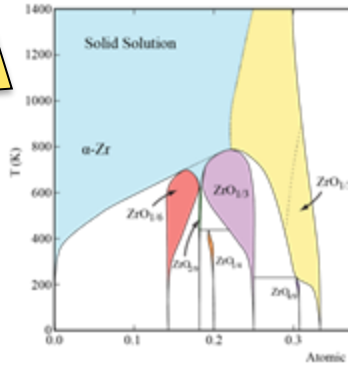
$$E(\vec{\sigma}) = V_o + \sum_i V_i \sigma_i + \sum_{i,j} V_{i,j} \sigma_i \sigma_j + \sum_{i,j,k} V_{i,j,k} \sigma_i \sigma_j \sigma_k + ..$$

Cluster expansion effective Hamiltonian (Clex)

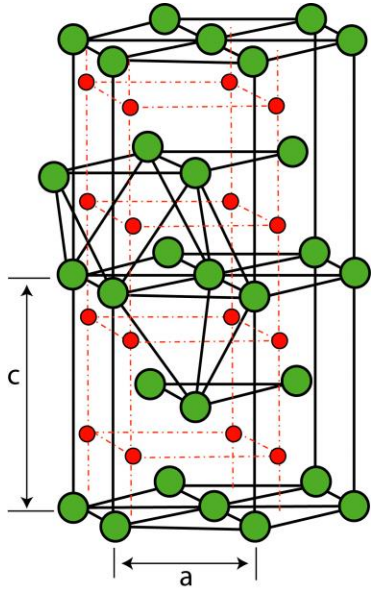
Monte Carlo Calculations



Free energy, Kinetic coef. vs x, T, σ, ...



Tutorial Project: Zr-O binary system



Zr:

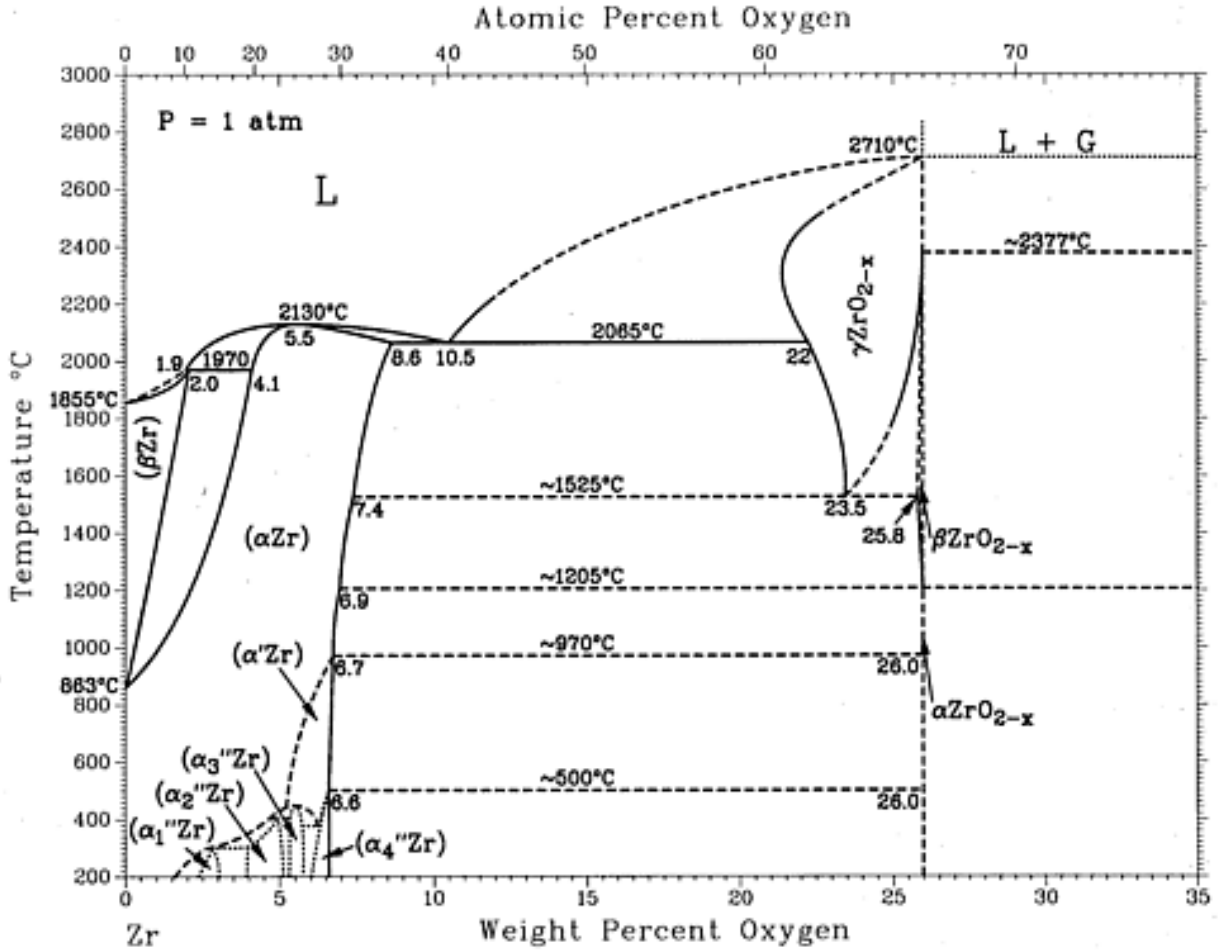
- Very high O solubility

ZrO_x

- Series of suboxide phases

ZrO_{2-x}

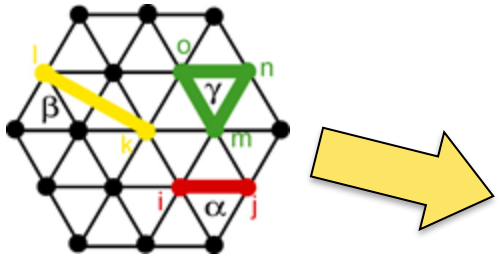
- Oxide



J.P. Abriata, J. Garcés, and R. Versaci, Bulletin of Alloy Phase Diagrams Vol. 7 No. 2 1986 .

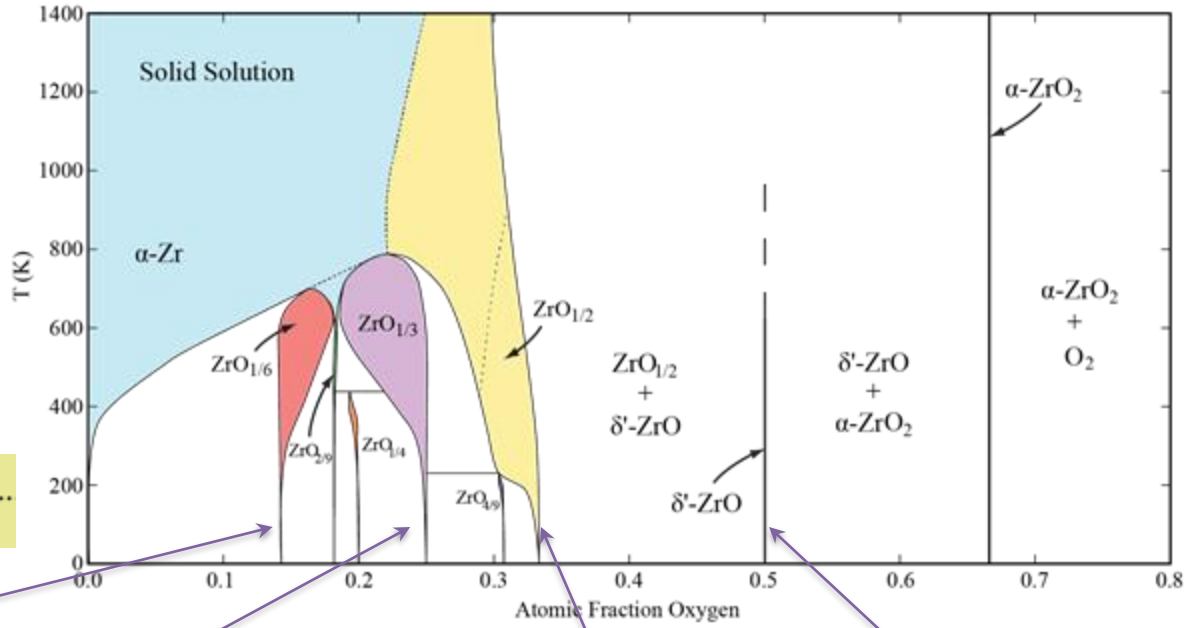
Configurational Cluster Expansion

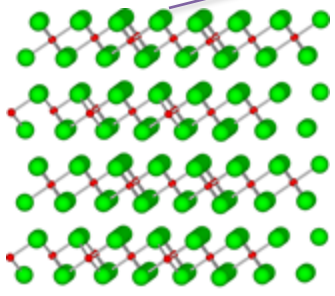
B. Puchala, A. Van der Ven, Physical Review B, 88, 094108 (2013).



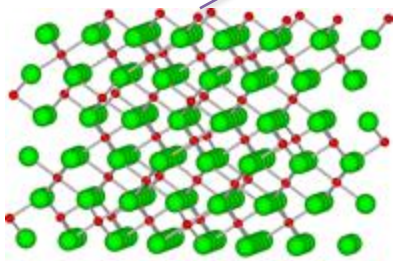
Configurational

$$E(\vec{\sigma}) = V_o + \sum_i V_i \sigma_i + \sum_{i,j} V_{i,j} \sigma_i \sigma_j + \sum_{i,j,k} V_{i,j,k} \sigma_i \sigma_j \sigma_k + ..$$

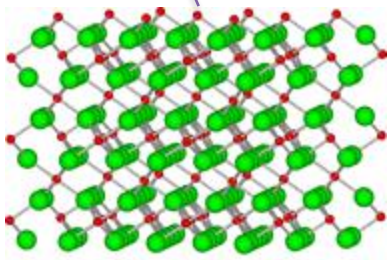




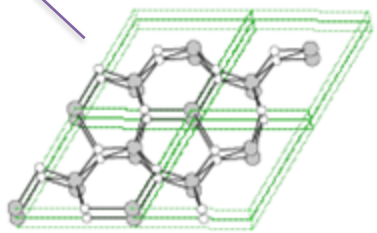
$ZrO_{1/}$



$ZrO_{1/3}$



$ZrO_{1/2}$



ZrO

B. Puchala, A. Van der Ven, Physical Review B, 88, 094108 (2013).