

10.675 LECTURE 24

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1. TODAY

Surface Phase Diagram

V,W interaction parameters

$E(p)$ where $p=1$ is occupied, $p=0$ is unoccupied

$$E(p) = V_o + \sum w_i p_i + \sum w_{ij} p_i p_j + \sum_{ijk} p_i p_j p_k$$

Where the w terms are the energetics between the set occupancies.

MC simulators to get convergence with NN energetic interactions.

NEB - Nudged Elastic Band

Change electronic Structure

→ alloys

→ strains

→ additives

→ steps

Weighted D-band analysis