Mike Payne 60<sup>th</sup>

Using DFT for predictive materials science by hook or by crook Gábor Csányi

### "Learn on the fly"

PHYSICAL REVIEW LETTERS

VOLUME 93, NUMBER 17

week ending 22 OCTOBER 2004

#### "Learn on the Fly": A Hybrid Classical and Quantum-Mechanical Molecular Dynamics Simulation

Gabor Csányi,<sup>1</sup> T. Albaret,<sup>3</sup> M. C. Payne,<sup>1</sup> and A. De Vita<sup>2,3</sup>

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"Real learning"

PRL 104, 136403 (2010)

PHYSICAL REVIEW LETTERS

week ending 2 APRIL 2010

#### Gaussian Approximation Potentials: The Accuracy of Quantum Mechanics, without the Electrons

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### Silicon - again



### Phase diagrams: Nested Sampling

#### PHYSICAL REVIEW B 93, 174108 (2016)

#### Determining pressure-temperature phase diagrams of materials

Robert J. N. Baldock,<sup>1,\*</sup> Lívia B. Pártay,<sup>2</sup> Albert P. Bartók,<sup>3</sup> Michael C. Payne,<sup>1</sup> and Gábor Csányi<sup>3</sup>
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Approximation of partition function  $\Delta(\beta, P, N)$  using cumulative density of states  $\chi$ 

$$\Delta(\beta, P, N) = \frac{\beta P}{N!} \left(\frac{2\pi m}{\beta h^2}\right)^{3N/2} \int_{-\infty}^{\infty} d\tilde{H} \frac{\partial \chi}{\partial \tilde{H}} e^{-\beta \tilde{H}}$$
$$\approx \frac{\beta P}{N!} \left(\frac{2\pi m}{\beta h^2}\right)^{3N/2} \sum_{i} (\chi_{i-1} - \chi_i) e^{-\beta \tilde{H}_i}$$

Isobaric heat capacity  $C_p$  to find first order phase transitions (e.g. liquid-solid, solid-solid)

$$C_P = k_B \beta^2 \frac{\partial^2 \log \Delta(\beta, P, N)}{\partial \beta^2}$$

'Top down' approach: 'High energy'  $\rightarrow$  Global minimum





# Phase diagrams: Nested Sampling











# Thanks Mike!

- Unwavering intellectual, material and social support for research
- Find the funding to do what you think should be done, rather than the other way around. And if you can't find it, do it anyway.
- Mike's enthusiasm is infectious, not just in science

