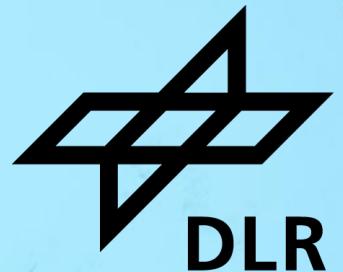


Materials Physics in the Quantum Realm

Matthias Sperl, DLR Institut für Materialphysik im Weltraum

Erik Schultheis, DLR Institut für Werkstoff-Forschung



ExaScale-Computer: 10^{18} Flops and 500 MEuro



Frontier in Oak Ridge National Laboratory, USA

Matthias Sperl, DLR-MP, 27. September 2023

Erster europäischer Exascale-Superrechner kommt nach Jülich

EuroHPC JU, das European High Performance Computing Joint Undertaking, wählt das Forschungszentrum Jülich als Partner im deutschen Gauss Centre for Supercomputing aus, um den ersten europäischen Supercomputer der nächsten Generation zu betreiben.

Jülich, 15. Juni 2022 – Die Entscheidung ist gefallen. Das Forschungszentrum Jülich wird Standort des ersten europäischen Exascale-Rechners. Der Supercomputer soll als erster Rechner in Europa die Grenze von 1 Trillion Rechenoperationen pro Sekunde – einer „1“ mit 18 Nullen – brechen. Beschafft werden soll das System von der europäischen Supercomputing-Initiative EuroHPC JU. Der Exascale-Rechner wird dazu beitragen, bedeutende und drängende wissenschaftliche Fragen zu lösen, etwa zum Klimawandel, zur Bewältigung von Pandemien und zur nachhaltigen Energieerzeugung, und den intensiven Einsatz von Künstlicher Intelligenz sowie die Analyse großer Datenmengen ermöglichen. Die Gesamtkosten für das System belaufen sich auf 500 Mio. Euro. 250 Mio. Euro werden von der europäischen Supercomputing-Initiative EuroHPC JU und 250 Mio. Euro zu gleichen Teilen vom Bundesministerium für Bildung und Forschung (BMBF) und dem Ministerium für Kultur und Wissenschaft des Landes Nordrhein-Westfalen (MKW NRW) getragen.



Deutschlands schnellster Superrechner JUWELS am Forschungszentrum Jülich, der über das Gauss Centre for Supercomputing (GCS) zu gleichen Teilen durch das Bundesministerium für Bildung und Forschung (BMBF) und das Ministerium für Kultur und Wissenschaft des Landes Nordrhein-Westfalen (MKW NRW) finanziert wird.
(Copyright: Forschungszentrum Jülich / Sascha Kreklau)

Der Rechner mit dem Namen JUPITER, die Abkürzung steht für „Joint Undertaking Pioneer for Innovative and Transformative Exascale Research“, wird ab 2023 in einem eigens dafür errichteten Gebäude auf dem Campus des

<https://top500.org/> - <https://www.olcf.ornl.gov/frontier/> -
<https://www.fz-juelich.de/de/aktuelles/news/pressemitteilungen/2022/exascale-standort-entscheidung>

Alternative Quantum Hardware

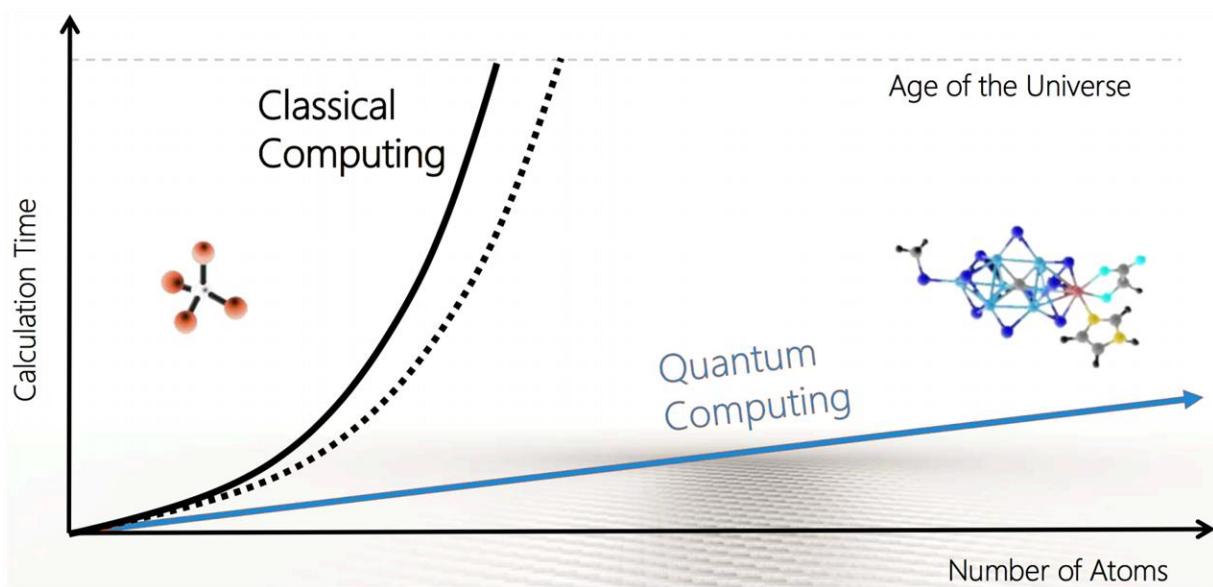


High Performance Computing
(HPC)



Exponential increase in computing time with atom number

Hybrid Simulations for Materials Science



Quantum Computing
(QC)



Near-linear increase in computing time with atom number

Quantum Computing and Machine Learning

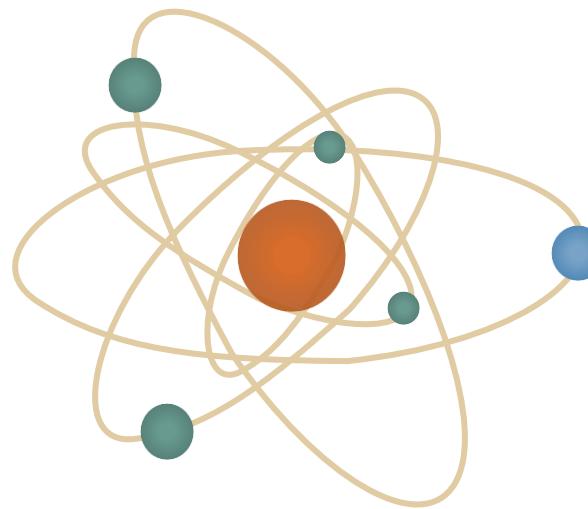


High Performance Computing
Classical algorithms



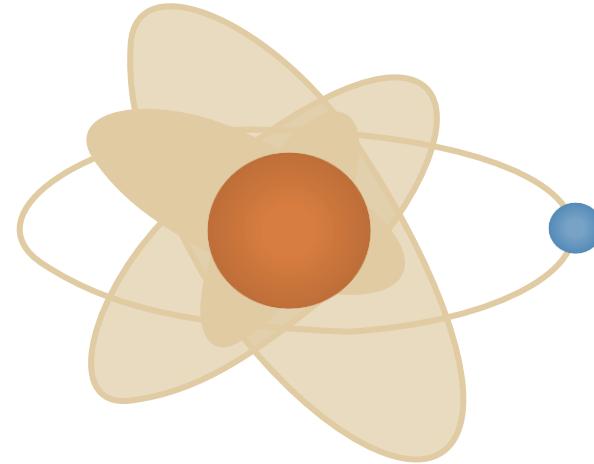
Exponential increase in com-
puting time with atom number

Schroedinger Equation



Accurate solution
limited to 10 atoms

Density Functional Theory



Approximation
limited to 1000 atoms

Simplified
simulations of
materials with
narrow composition
range

Approximation
causes moderate
simulation quality

Quantum Computing and Machine Learning

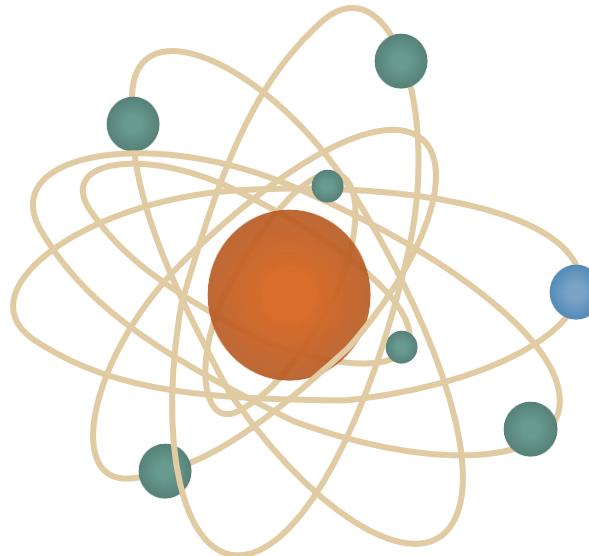


Quantum Computing
Quantum algorithms



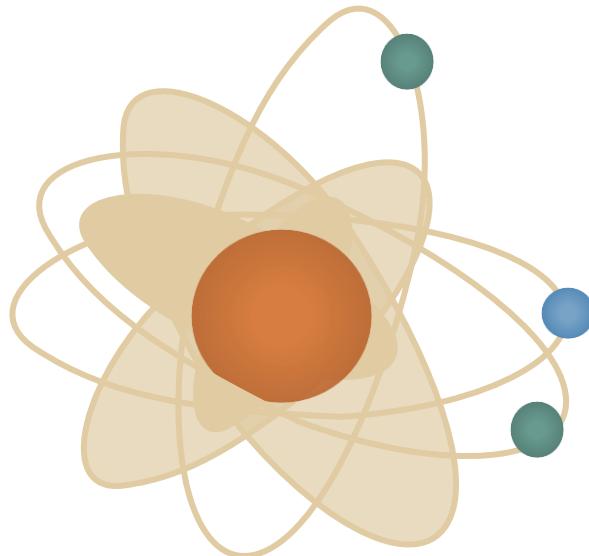
Near-linear increase in com-
puting time with atom number

Schroedinger Equation



Accurate solution
 $>> 10$ atoms

Hybrid Schroedinger-Density-
Functional Theory solution



Hybrid accurate solution
 $>> 1000$ atoms

Full simulation of
complex metal alloys
and polymers

High fidelity
simulation quality

New Materials from Multiple Components: Many Possible Combinations



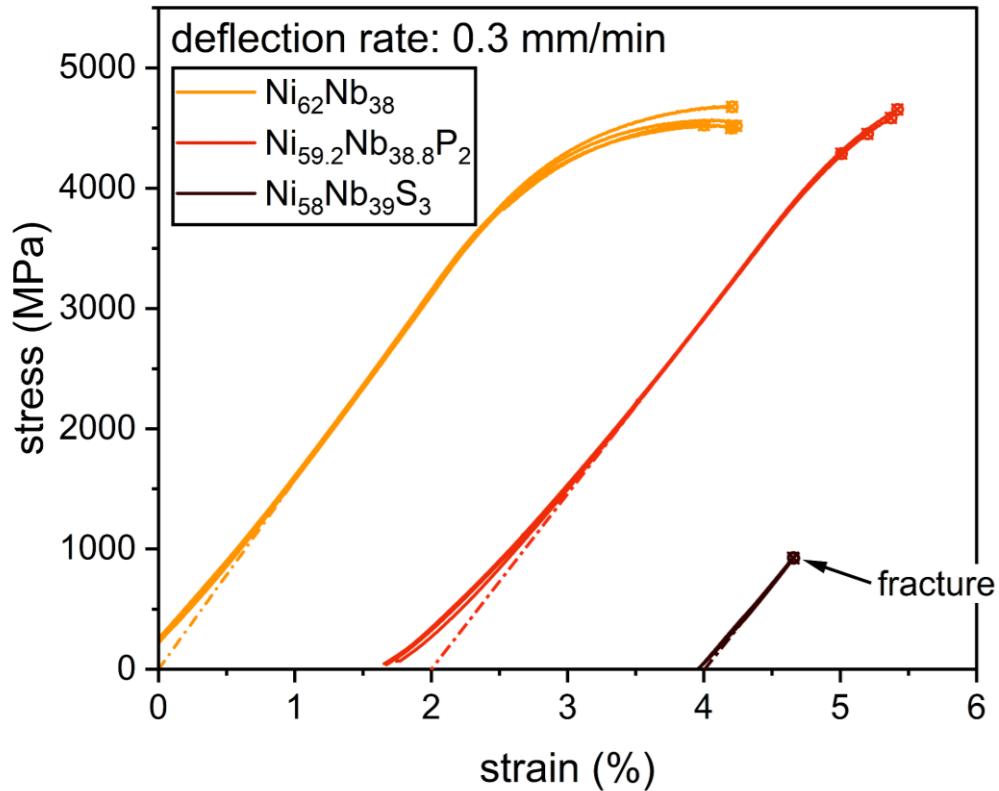
1 H																									2 He
3 Li		4 Be																							9 F
11 Na		12 Mg																							10 Ne
19 K		20 Ca	21 Sc		22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr						
37 Rb		38 Sr	39 Y		40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe						
55 Cs		56 Ba	57 La	*	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn						
87 Fr		88 Ra	89 Ac	*	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Nh	114 Fl	115 Mc	116 Lv	117 Ts	118 Og						

Sustainable alloy development

50-60 frequently used elements → 10^{60} possible combinations

Small Contributions Matter

Defects, Doping, Glass-Ceramics, Glass-Forming Ability, ...



- Small changes can have big impacts, cf. mechanical properties
- Electronic structure changes structural properties
- Typically far less than 1 atom per unit cell
- No real definition of a unit cell for glasses

N. Grund, DLR-MP, Impact of Minor Additions on the Structure and Dynamics of Metallic Melts (2023) ; [Rusch et al., Ni-Nb-P-based bulk glass-forming alloys: Superior material properties combined in one alloy family, Acta Mat. 254, 118968 \(2023\).](#)

Complex Routes to a Material: Glasses, Glass-Ceramics, and their dynamics

J. Deubener et al.

Journal of Non-Crystalline Solids 501 (2018) 3–10

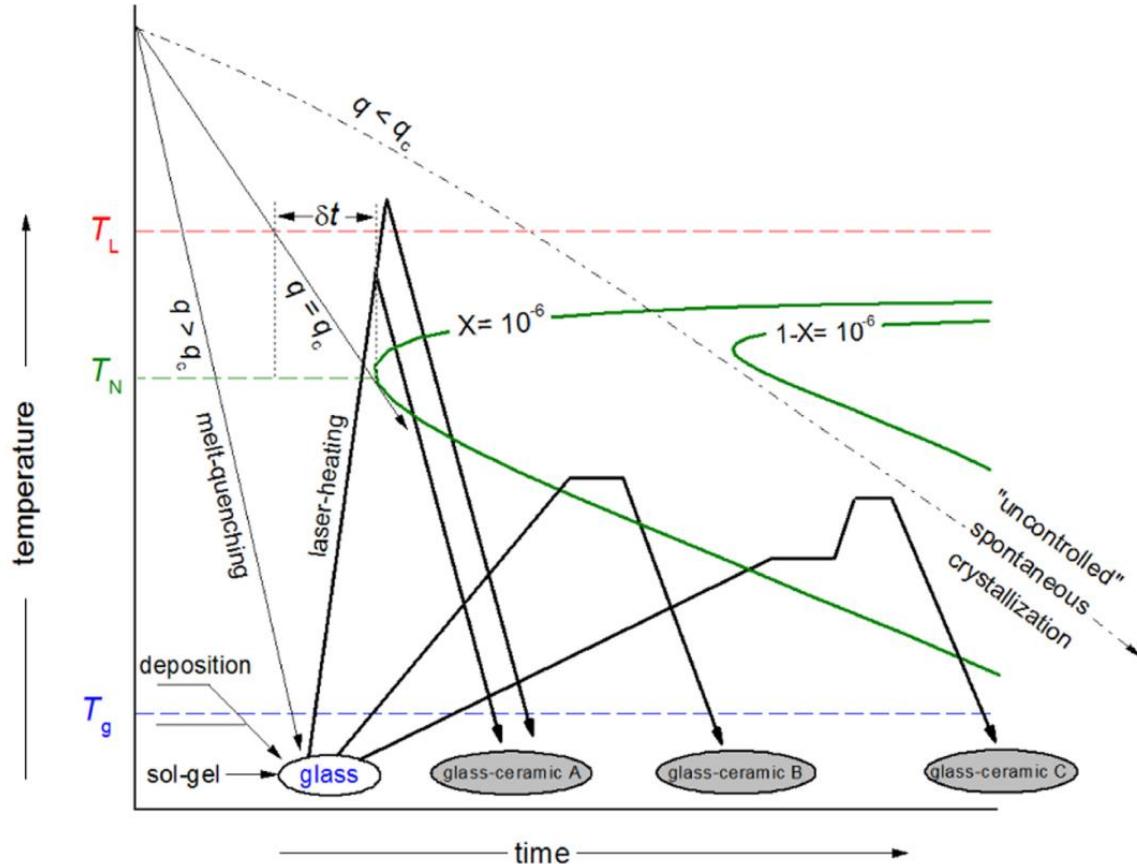


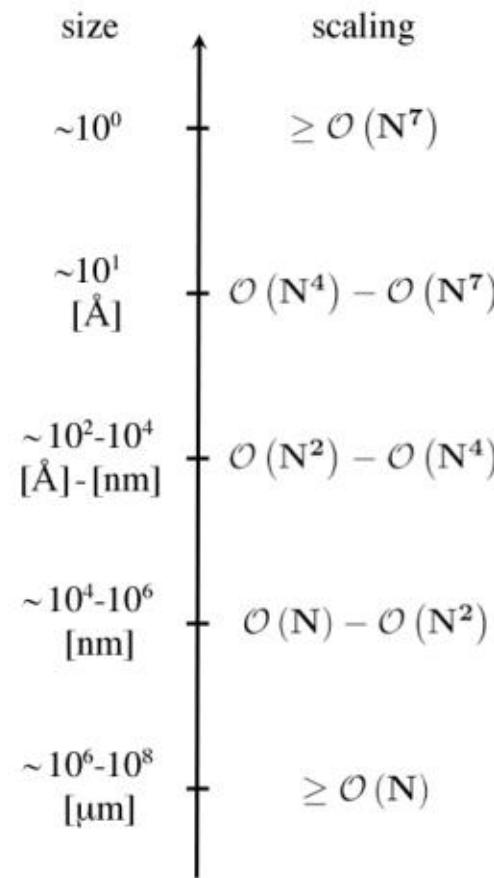
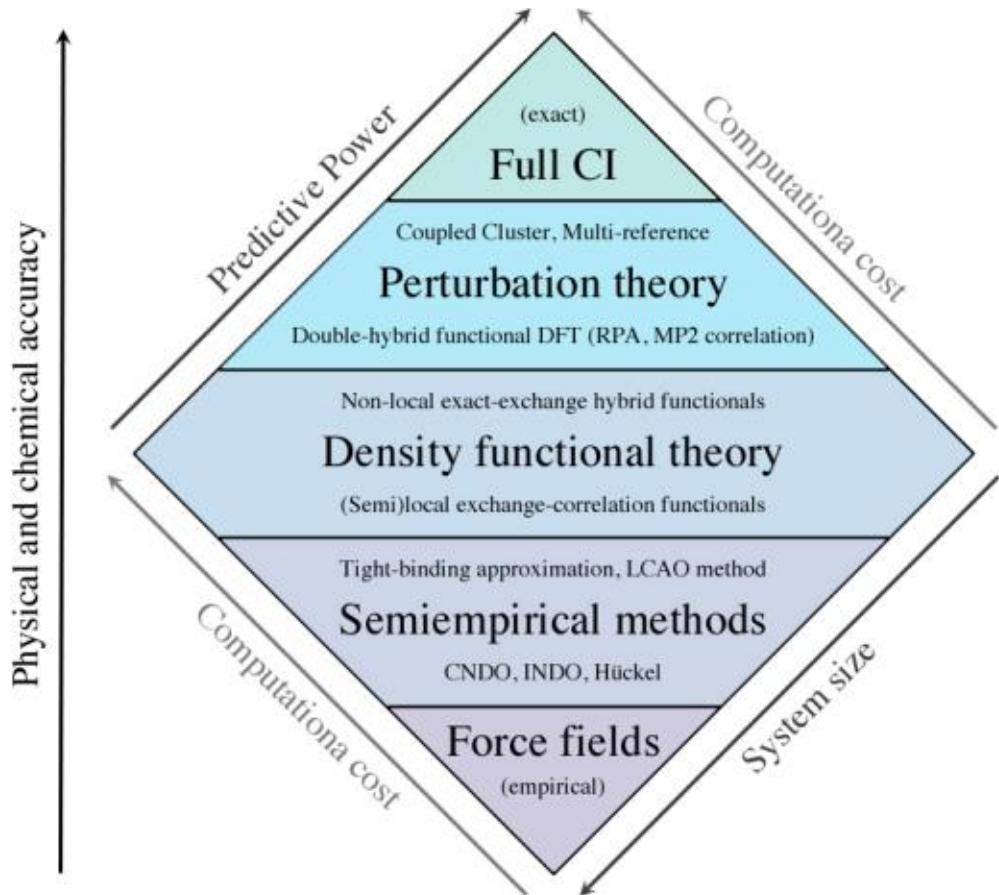
Fig. 1. Schematic description of the conversion of a glass into a glass-ceramic. The critical cooling rate is $q_c = (T_L - T_N) / \delta t$ with T_L = liquidus temperature, and T_N = "nose temperature" (=temperature at which the time δt to achieve a crystal fraction of 10^{-6} is shortest, according to Eq. (1)). Glass formation by melt-quenching takes place for $q \geq q_c$. "Uncontrolled" spontaneous crystallization occurs for $q < q_c$. The glass-ceramic A is obtained during cooling, whereas glass-ceramics B and C are converted by single and double-stage heat-treatments, respectively.

- Multiple steps in processes
- Amorphous and crystalline states
- Zerodur, Schott (1968)
- Ceran, Schott (1971)



[J. Deubner, et al., Updated definition of glass-ceramics, J. Non-Cryst. Solids 501, 3 \(2018\).](#)

Computational Costs and Predictive Power: Reassessment of Scalings

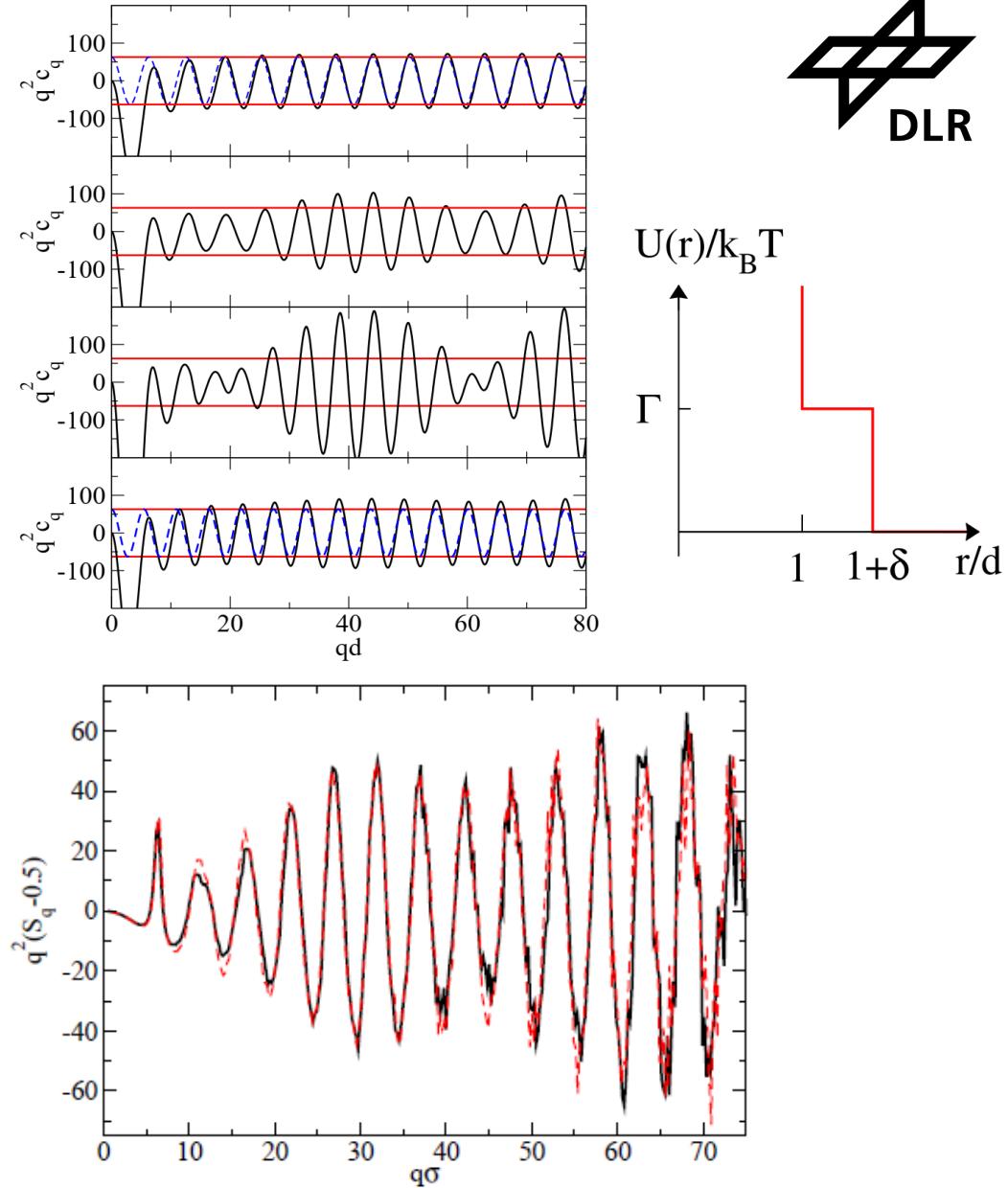
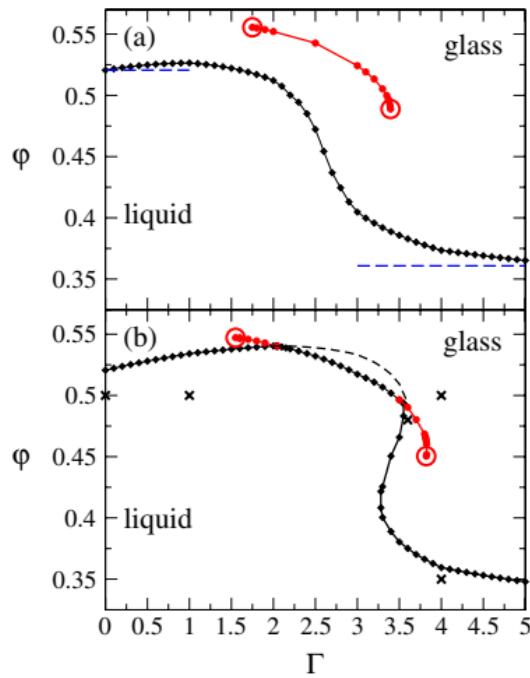
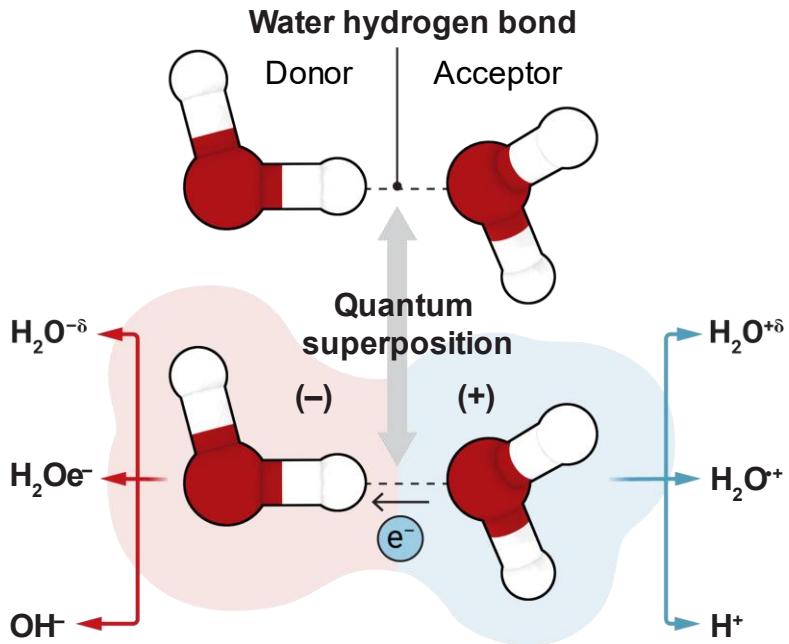


- Test of classical approximations
- Invention of novel approximations
- Application-specific optimum

Marc Landmann, *Fingerprints of Order and Disorder*,
Dissertation Uni Paderborn, p83, (2020)

Extension of Theory

- Simple models with complex effects: What about realistic models?
- Novel state/phase transitions
- Orders of magnitude changes in material properties

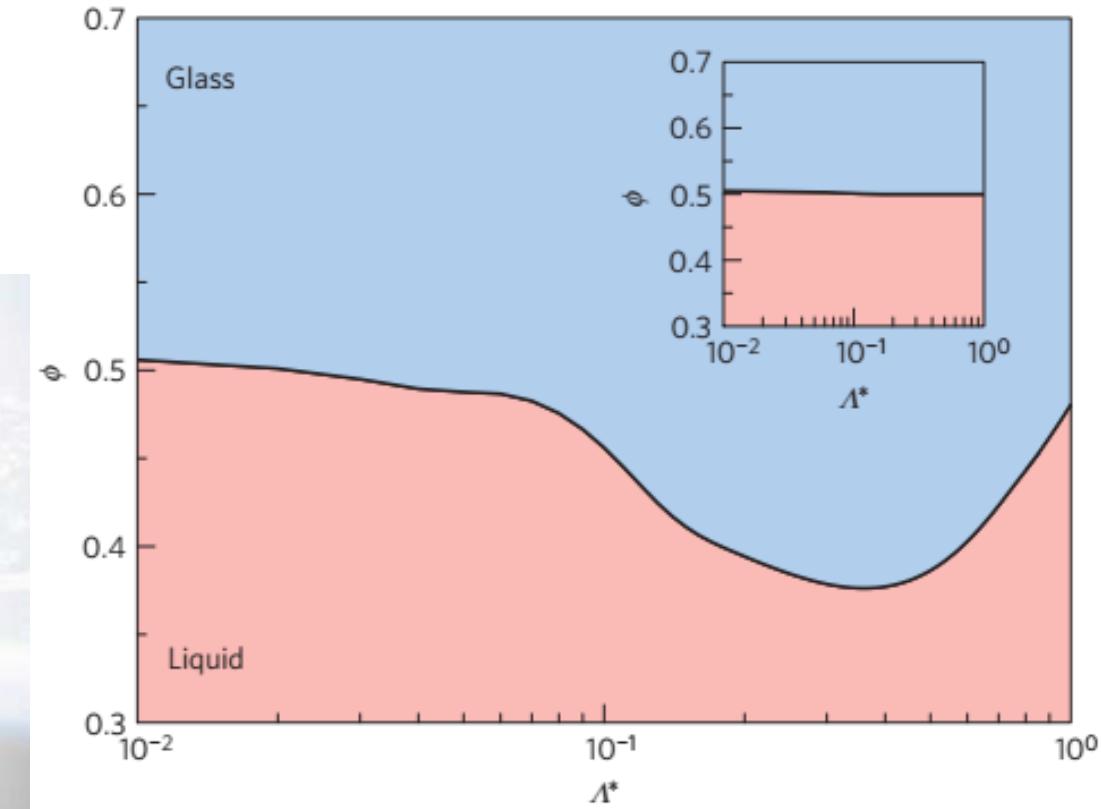
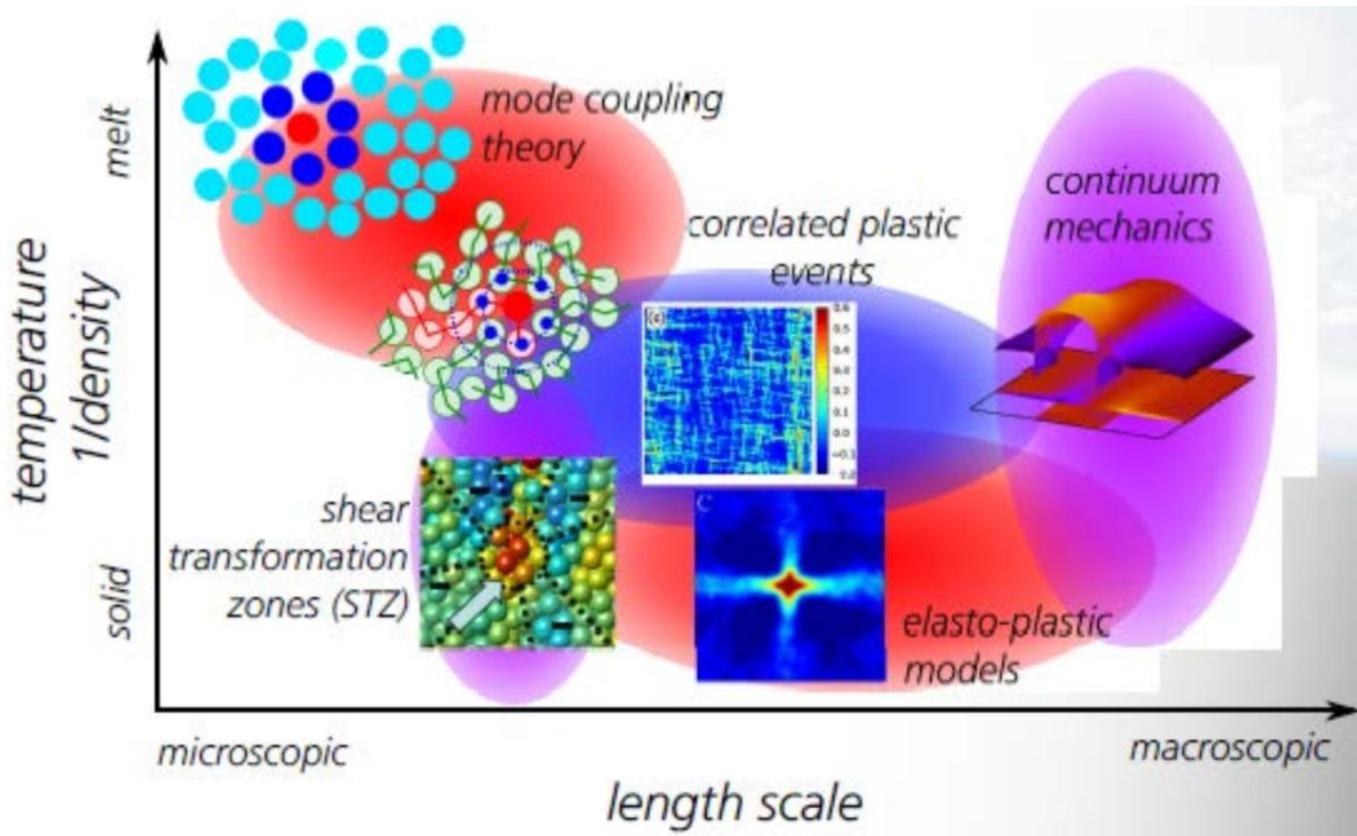


[Dor Ben-Amotz Science 376, 800\(2022\)](#). [M.Sperl, et. al., Phys. Rev. Lett. 104, 145701 \(2010\)](#).
[N. Gnan, et al., Phys. Rev. Lett. 113, 258302 \(2014\)](#).

Materials Physics: Theory, Simulation and Experiments



- Crossing different scales of description
- Experimental data from laboratory and space



- Simple models with quantum effects
- Hard-Sphere System: glass transitions
- Landscape for (quantum) machine learning

Water, Metallic Alloys, Concrete and Redox Materials



Metallic Alloys and Redox Materials: Many possible combinations; Small contributions matter

Minerals: Structure and dynamics determine properties and processes

Theory: Hints to quantum effects and influences



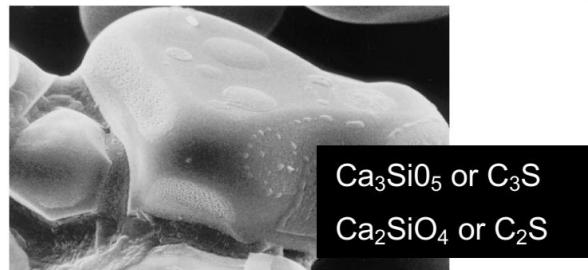
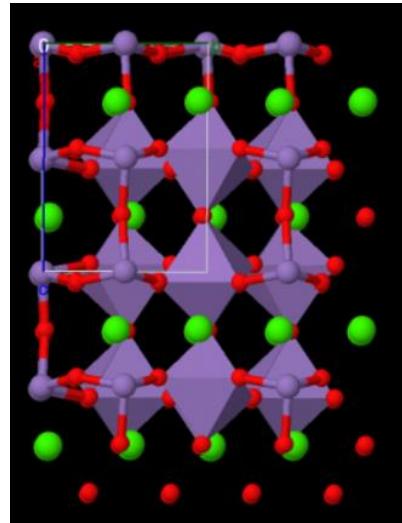
PROJEKT DER UNI KÖLN SOLL
KLIMASCHUTZ UNTERSTÜTZEN

Astro-Matthias
erforscht Beton auf
der ISS



Matthias Maurer ist Werkstoffkundler und Astronaut

Foto: ESA



Ca_3SiO_5 or C_3S
 Ca_2SiO_4 or C_2S

10 μm

