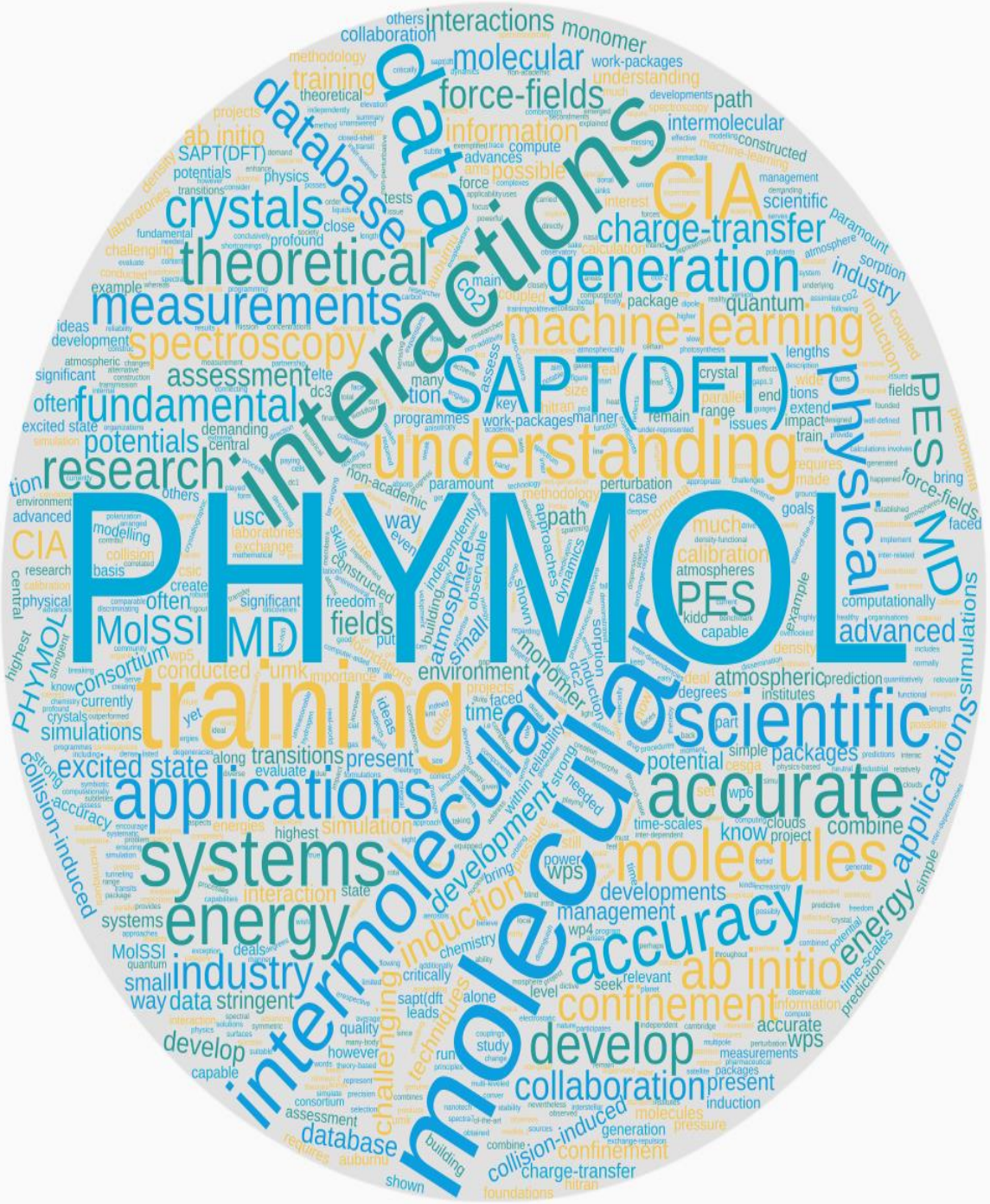
PHYMOL

CSÁSZÁR ATTILA

MOLEKULASZERKEZET ÉS DINAMIKA LABORATÓRIUM

& MTA-ELTE KOMPLEX KÉMIAI RENDSZEREK KUTATÓCSOPORT

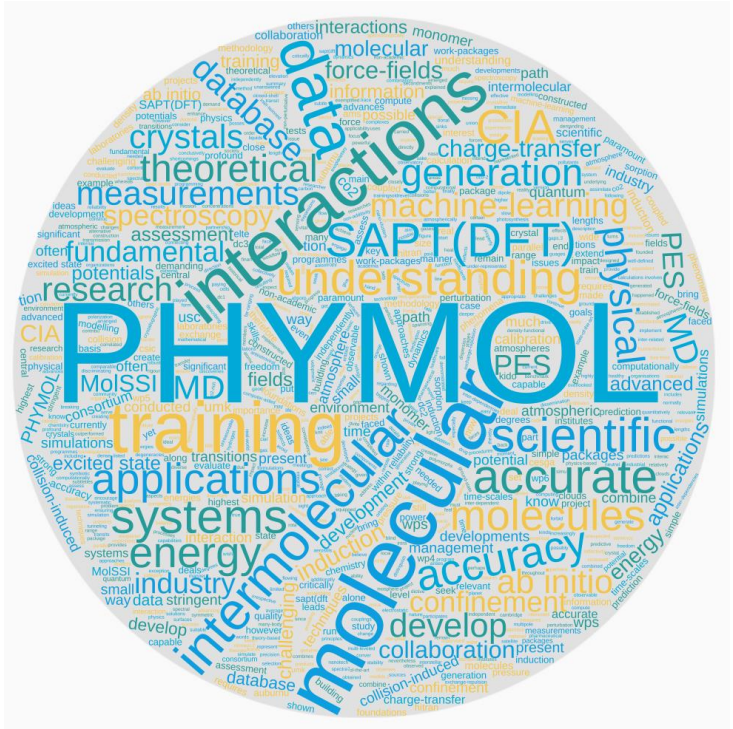
ELTE KÉMIAI INTÉZET



PHYMOL

Physics, Accuracy and Machine Learning:

Towards the next generation of Molecular Potentials



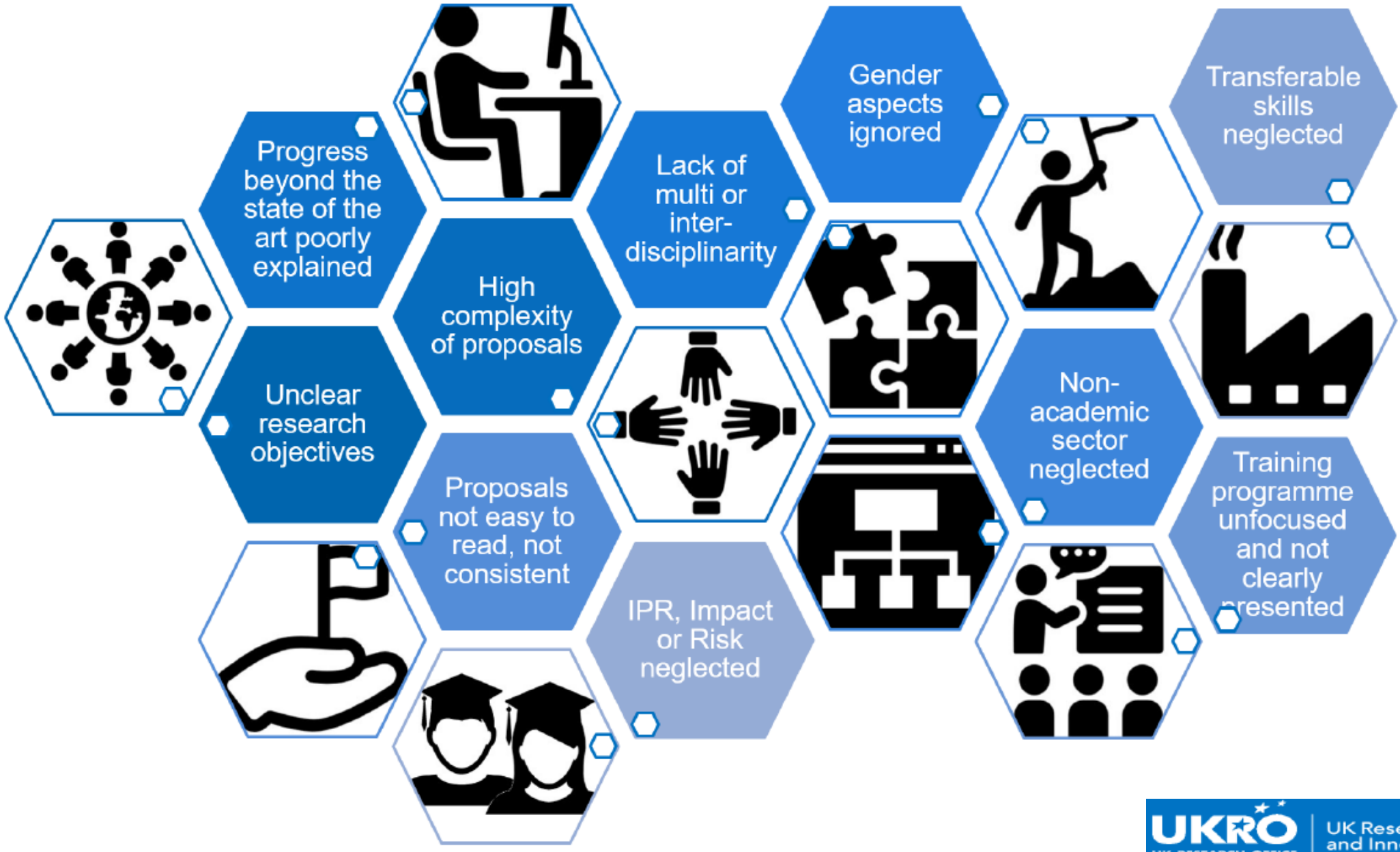
MSCA Key Features

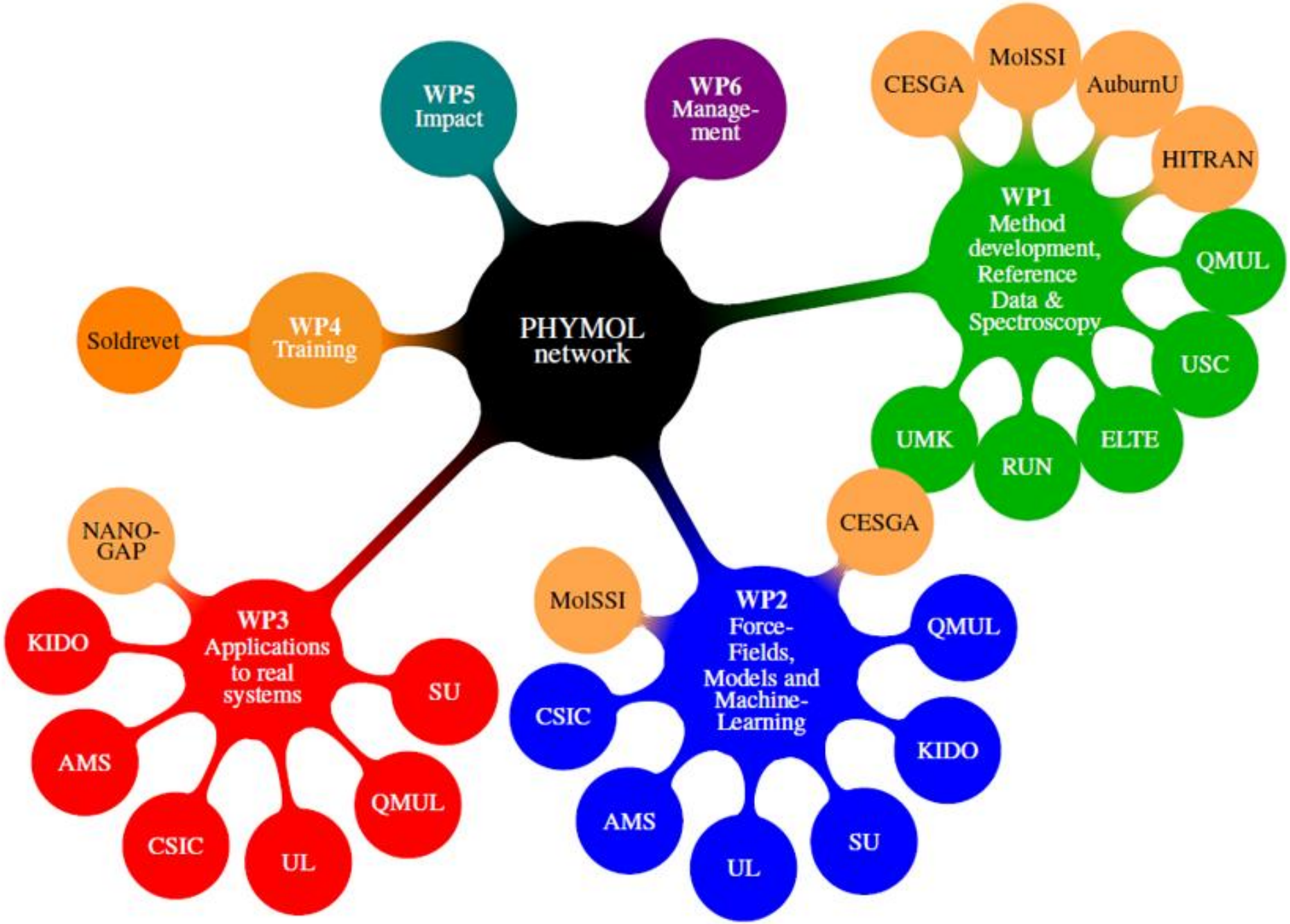
- Operates on a '**bottom-up**' basis
- For any research and innovation ideas (basic research; market take-up)
- **Mobility** (cross-border and cross-sector) is a key requirement
- Enhance skills of **people behind research and innovation**
- Strong participation across sectors
- Dissemination and **public engagement** - public outreach
- **Gender Friendly and Inclusive** – equal opportunities in the research content

ITN Evaluation Criteria

Excellence	Impact	Quality and efficiency of the implementation
Quality and pertinence of the project's research and innovation objectives (and the extent to which they are ambitious, and go beyond the state of the art)	Contribution to structuring doctoral training at the European level and to strengthening European innovation capacity, including the potential for: a) meaningful contribution of the non-academic sector to the doctoral training, as appropriate to the implementation mode and research field b) developing sustainable elements of doctoral programme	Quality and effectiveness of the work plan, assessment of risks and appropriateness of the effort assigned to work packages
Soundness of the proposed methodology (including interdisciplinary approaches, consideration of the gender dimension and other diversity aspects if relevant for the research project, and the quality and appropriateness of open science practices)	Suitability and quality of the measures to maximise expected outcomes and impacts, as set out in the dissemination and exploitation plan, including communication activities	Quality, capacity and role of each participant, including hosting arrangements and extent to which the consortium as a whole brings together the necessary expertise
Quality and credibility of the training programme (including transferable skills, inter/multidisciplinary, inter-sectoral and gender as well as other diversity aspects)	Credibility of the measures to enhance the career perspectives and employability of researchers and contribution to their skills development	
Quality of the supervision (including mandatory joint supervision for industrial and joint doctorate projects)	The magnitude and importance of the project's contribution to the expected scientific, societal and economic impacts	

Avoid the Pitfalls




PHYMOL network
WP1 Method development, Reference Data & Spectroscopy
CESGA
MolSSI
AuburnU
HITRAN
QMUL
USC
ELTE
RUN
UMK
WP2 Force-Fields, Models and Machine-Learning
CESGA
MolSSI
QMUL
KIDO
SU
UL
AMS
CSIC
WP3 Applications to real systems
NANO-GAP
KIDO
SU
QMUL
UL
CSIC
AMS
WP4 Training
Soldrevet
WP5 Impact
WP6 Manage-ment

A konzorcium összetétele – Akadémiai tagok

- QMUL: Queen Mary University (UK)
- ELTE: Eötvös Loránd University (HU)
- USC: Universidad de Santiago de Compostela (ES)
- UL: Université du Luxembourg (LU)
- RUN: Stichting Radboud Universiteit (NL)
- UMK: Uniwersytet Mikolaja Kopernika w Toruniu (PL)
- CSIC: Agencia Estatal Consejo Superior de Investigaciones Cientificas (ES)
- SU: Sorbonne Universite (FR)

A konzorcium összetétele – Kedvezményezettek

- AMS: Avant-garde Materials Simulations Deutschland GmbH (DE)
- KIDO: KIDO Dynamics SA (ES)

A konzorcium összetétele – Partnerek

- MolSSI: The Molecular Sciences Software Institute (US)
- AuburnU: Auburn University (US)
- HITRAN: High-Resolution Transmission Molecular Absorption Database (US)
- NANOGAP: NANOGAP (ES)
- CESGA: Fundación Pública Galega Centro Tecnolóxico de Supercomputación de Galicia (ES)
- Soldrevet: Soldrevet Chemistry (NO)

Excellence

PHYMOL:
Physics, Accuracy and Machine Learning: Towards the next-generation of Molecular Potentials

Summary: *In the* **PHYMOL** *collaboration we bring together leading experts in the fields of molecular simulations, quantum chemistry, crystal structure prediction, intermolecular modelling, spectroscopy, machine-learning, and nano-clusters, from* **12 academic** *institutes and national laboratories, and* **4 industrial** *entities, in an ambitious programme of research and training to develop a new generation of researchers in the field of molecular modelling.* **PHYMOL** *combines the most advanced* **physical understanding** *of molecular interactions with* **machine-learning** *in a symbiotic manner that will lead to a new generation of researches capable of advancing solutions to problems of importance in healthcare, energy and the environment, as well as basic science. The private sector is an integral part of* **PHYMOL** *and participates in management, training and research. With this union of forces from academia, industry from the EU and the US, we seek to keep molecular simulation techniques at the fore-front of industry and science in the EU.*

of this consortium: *In one sentence, PHYMOL describes our quest to train a new generation of researchers to develop accurate physical models, to enhance our theoretical methods, and to combine them with advanced machine-learning technology, so as to be able to develop a new generation of molecular potentials that can quantitatively and reliably address some of the more challenging applications we face.*

Structure

WP No.	WP Title	Lead Ben. No.	Start Month	End Month	Activity Type	Lead Beneficiary Short Name	DC Involvment
1	Generation and assessment of reference data	B4	8	48	**R, T**	RUN	DC1, DC2, & DC3
2	Force-Fields and Machine-Learning	B7	8	48	**R, T**	SU	DC4, DC5, DC6, & DC7.
3	Applications of the models	B3	8	48	**R, T**	UL	DC6, DC7, DC8, DC9 & DC10.
4	Training	B2	8	48	**T**	USC	All
5	Impact	B5	8	48	**C, D**	UMK	All
6	Management	B1	1	48	**M**	QMUL	All

Table 1.1a: Work package list. **R**= Research, **T**= Training, **M**= Management, **C**= Communication, **D**= Dissemination.

List of partners for the **DN** network. The roles of the partners can be **S** = Secondment, **T** = Training, **Co** = PhD Co-Supervision, **M** = PhD Mentor

Evaluation summary - PHYMOL

Evaluation Result

Total score: 94.20% (Threshold: 70/100.00)

Criterion 1 - Excellence

Score: **4.60** (Threshold: 3/5.00 , Weight: 50.00%)

Criterion 2 - Impact

Score: **4.70** (Threshold: 3/5.00 , Weight: 30.00%)

Criterion 3 - implementation

Score: **5.00** (Threshold: 3/5.00 , Weight: 20.00%)