PRACE-Proje Çağrıları Bilgi Günü
DECI Çağrıları

Adem Tekin

İTÜ Bilişim Enstitüsü, Hesaplamalı Bilim ve Mühendislik Anabilim Dalı

PRACE | nedir

- AB bilim adamları ve araştırmacılarına birinci-sınıf HPC sistemlerine açık erişim
- Farklı bilimsel alanları desteklemek için çeşitli mimariler
- Bilimsel mükemmelliği teşvik için Avrupa düzeyinde hakem değerlendirmesi
- Ulusal hükümetler ve Avrupa Komisyonu (EC) tarafından desteklenen sağlam ve kalıcı bir HPC finansman planı
- Avrupa'nın endüstriyel HPC kullanıcıları ve tedarikçileriyle işbirliği imkanı

PRACE | başarılar

- 687 bilimsel proje desteklendi
- 110 Petaflops of peak performance on 7 Tier-0 systems
- >21 milyar 2010'dan itibaren - %63 Avrupa dışı yürütücü
- >50 firma desteklendi
- >12 000 kişi PRACE Training ile eğitim gördü

PRACE | Tier-0 Systems 2018

NEW ENTRY 2018
JUWELS (Module 1): Bull Sequana
GAUSS @ FZJ, Jülich, Germany
#26 Top 500

MareNostrum: IBM
BSC, Barcelona, Spain
#25 Top 500

Piz Daint: Cray XC50
CSCS, Lugano, Switzerland
#5 Top 500

NEW ENTRY 2018/2019
SuperMUC NG : Lenovo cluster GAUSS @ LRZ, Garching, Germany #8 Top 500

NEW ENTRY 2018
JOLIOT CURIE : Bull Sequana
GENCI/CEA, Bruyères-le-Châtel, France #40 Top 500

MARCONI: Lenovo
CINECA, Bologna, Italy
#19 Top 500

Hazel Hen: Cray
GAUSS/HLRS, Stuttgart, Germany
#30 Top 500

Close to 110 Petaflops cumulated peak performance

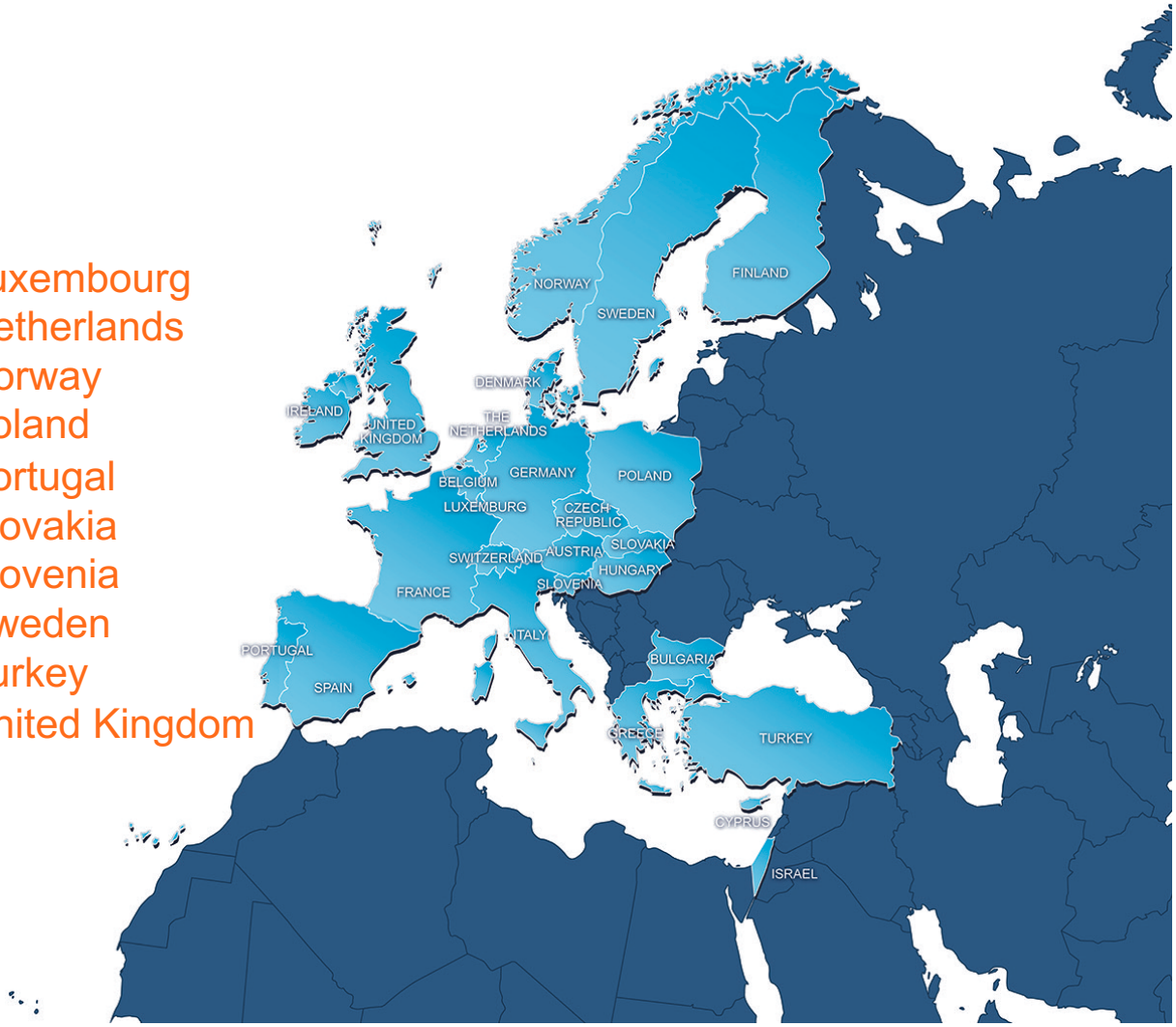
PRACE | üyeler

Hosting Üyeler

- France
- Germany
- Italy
- Spain
- Switzerland

Genel Üyeler (PRACE 2)

- Austria
- Belgium
- Bulgaria
- Cyprus
- Czech Republic
- Denmark
- Finland
- Greece
- Hungary
- Ireland
- Israel
- Luxembourg
- Netherlands
- Norway
- Poland
- Portugal
- Slovakia
- Slovenia
- Sweden
- Turkey
- United Kingdom



PRACE | mevcut hizmetler

Erişim

Tier-0 sistemleri
- Project Access
  1-3 yıl
- Preparatory Access
  Type A, B, C, D

Tier-1 sistemleri
- DECI Programı

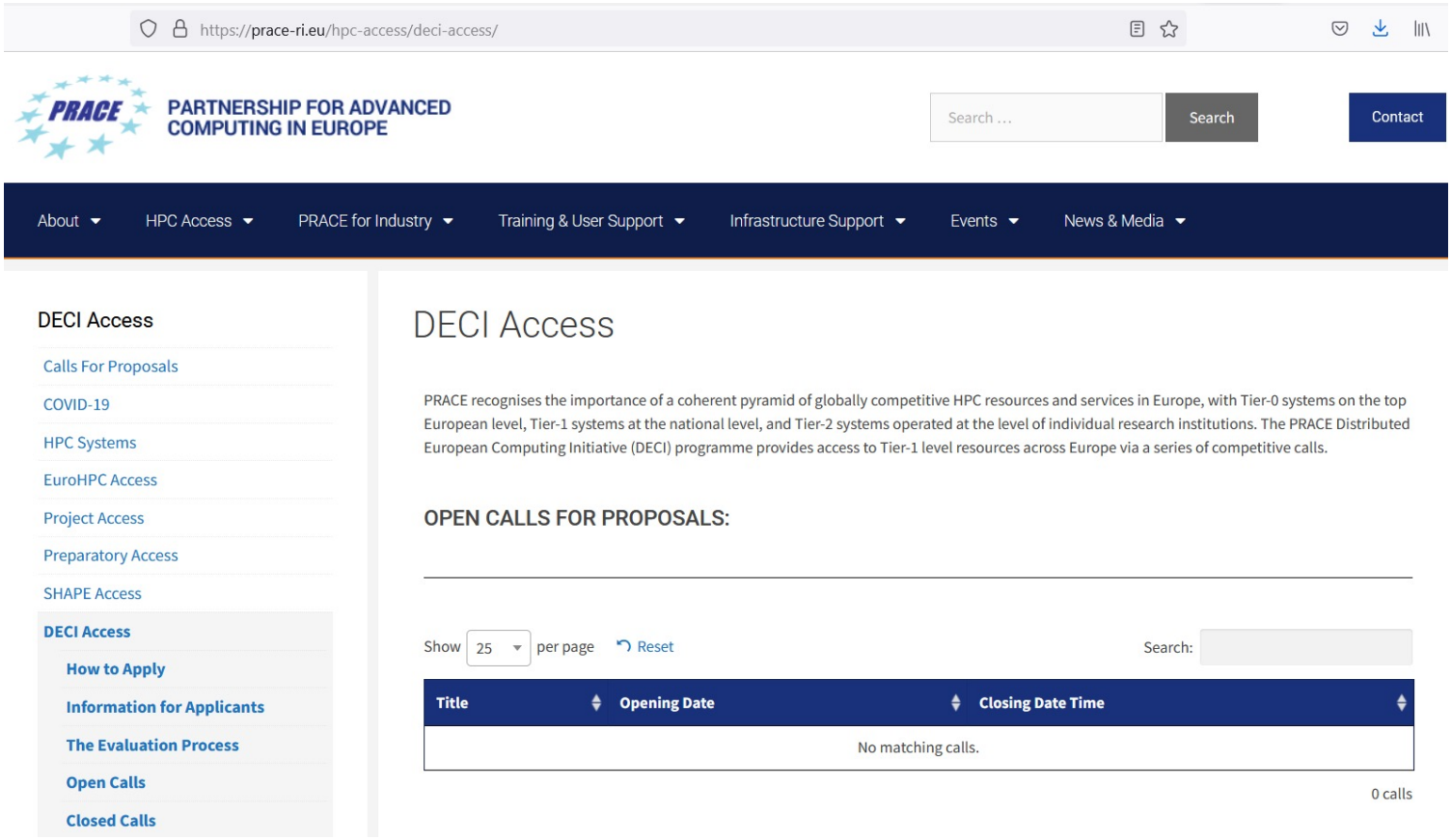
Destek

Uygulama Etkinleştirme & Destek
- Preparatory access Type C
- Preparatory access Type D
  - Tier-1 for Tier-0
- SHAPE
- HLST desteği

Eğitim
- Eğitim Portalı
- PATC, PTC
- Sezonluk okullar
- Uluslararası HPC Yaz Okulu
- MOOC

- Code Vault
- En iyi Uygulama Kılavuzları
- White Papers

PRACE | https://prace-ri.eu/hpc-access/deci-access/



PRACE | DECI Programı

- Avrupa Tier 1 HPC kaynaklarına (ulusal sistemler) uluslararası erişim sağlar
- Projelerin Tier 0 HPC kaynaklarının kullanılmasına gereksinimi bulunmamalıdır
- Başarılı projeler için 12 aylık HPC hesaplama kaynağı sunar
- Çeşitli mimarilerdeki hesaplama kaynakları PRACE ortakları tarafından sağlanır
- Başvuru sahiplerinin belirli bir makine veya mimari belirtmelerine gerek yoktur, fakat gerektiğinde destek verilebilir
- Verilen kaynak en fazla 5 milyon makine saatidir (ortalama 2.5 milyon makine saati)

PRACE | DECI için uygunluk

- Akademi ve endüstriden gelen proje başvuruları uygundur
- Proje yürütücüleri genel olarak akademik kuruluşlarda çalışırlar
- Bazı HPC merkezlerinde makinaların kimlerin tarafından kullanılmasını belirlemede farklı kısıtlarda (örneğin ABD ihracat kuralları gereği) bulunabilir

DECI | nasıl başvurulur

- Başvuru sahiplerini başvurularını https://deci-peer-review.cines.fr/ adresi üzerinden gönderebilirler
- Ancak açık bir çağrı varsa başvuru yapılabilir
- Açık çağrılar https://prace-ri.eu/hpc-access/deci-access/deci-access-open-calls/ adresinden kontrol edilebilir
- Proje başvuru aşamasında ortaya çıkabilecek problemler için deci-support(at)prace-ri.eu adresine eposta gönderilebilinir

DECI | değerlendirme aşaması

- Proje gönderimi: aynı projeye ait proje başvuru formu son başvuru tarihine kadar birçok kez gönderilebilir. Online doldurulacak proje başvuru formuna ilaveten projenin daha detaylı bir halde Word formunda hazırlanmalıdır.

- Ev sahibi HPC merkezinin atanması: proje yürütücüsü DECI çağrılarına kaynak sağlayan bir merkezden olmalı ve ev sahibi merkez DECI programına kaynak katkısı yapmalıdır. Proje önerisi ev sahibi merkeze atanır. Dış projeler (DECI programına kaynak katkısında bulunmayan bir ülkenin yürütücüsü) ise DECI merkezlerinden uygun olan birisine atanır.

DECI | değerlendirme aşaması

- İdari değerlendirme: ev sahibi merkez başvuruda ki girilen bilgilerin tutarlığını ve eksik olup olmadığını kontrol eder. Eksiklik olması durumunda, yürütücüyle iletişime geçebilir. Sonrasında, başvuru sahiplerine başvurularının doğru bir şekilde sunulduğunu ve uygunluk kriterlerini karşıladıklarına dair bir onay gönderilir.
- Teknik değerlendirme: başvuru ev sahibi merkezde ki bir teknik uzman tarafından teknik gereksinimlerin DECI'nin beklentilerini karşılayıp karşılamadığını kontrol eder. **Bu noktada önemli olan kullanılması düşünülen yazılımların istenen kaynakta ölçeklenebilir olmasıdır**. Teknik değerlendirme de önerilen mimarinin uygun olup olmadığı da kontrol edilir.

DECI | değerlendirme aşaması

- Bilimsel değerlendirme: yürütücünün başvurduğu ülkeden toplanan ulusal uzmanlar paneli tarafından projenin bilimsel incelemesi yapılır. Dış projelerse, Tier-0 kaynakları olan Avrupa ülkelerinin ki hakemlerce yapılır. Bazen, iç projeler de Tier-0 hakem havuzu tarafından gözden geçirilebilir. **Hakemler, projeleri bilimsel mükemmelliğe dayalı olarak sıralarlar.**
- Destekleme: DECI komitesi bilimsel mükemmellik temel ilke alınarak hangi projelerin desteklenmesi karar vermek için toplanır. Kaynak dağıtımında her ülke yaklaşık olarak katkıda bulunduğu kaynak kadar destek alır. Dış projeler içinse ev sahibi kaynakların %30'a kadar olan bir bölümü ayrılır.

DECI | değerlendirme aşaması

- Kaynak tahsisi: her başvurunun teknik gereksinimleri dikkate alınarak, projenin yürütüleceği DECI Tier-1 makinası atanır. Sonrasında, başvuru sahiplerine hesaplama tahsis ve atanan makinalar hakkında bilgi verilir ve kendilerinin desteği kabul edip etmediklerini teyit etmeleri istenir.

- Proje ömrü: yürütücülerin bir uzatma talebinde bulunmadıkları durumda, projeler bitiş tarihinde sona erer. Gerektiğinde, proje birkaç hafta daha uzatılabilir. Her projenin sonunda bir proje sonuç raporunun DECI'ye sunulması gerekmektedir.

DECI | değerlendirme aşaması

- Raporlama: DECI başarısını vurgulamak için, proje sonuç raporlarının analizine dayanarak, bazı proje sonuçlarının web sitelerinde yayınlayabilirler.

DECI | peer review tool
https://deci-peer-review.cines.fr

General information

Type of proposal: DECI 16th Project

Project title ■ 2D Crystal Structure Prediction of DNA base Self-Assemblies

Project acronym ■ 2DCSP (max. 15 characters)

Research field Materials Science

Detailled project document ■ DECI_16th_detailed_project_document_Adem_Tekin.pdf

DECI | peer review tool

Contact person for all correspondence

If different from the project leader below. *The project leader and the contact person will both receive all information.*
Please give your professional e-mail address.

Name :	Adem Tekin
Email address :	adem.tekin@be.itu.edu.tr
Organisation :	Istanbul Technical University, Informatics Institute

Project leader (personal data and contact)

Abstract of the project

If the project is successful this will be published on the PRACE website unless you mark it as confidential below. Please make this summary understandable to a general audience. (Maximum 500 words)

DECI | peer review tool

Further details (codes)

NOTE: If multiple codes are to be used, please give the specifications for each of them. Please visit the **"Edit codes"** section from the frontpage where you can add more codes.

We are interested in each of the codes you intend to run. Please provide the following details for **each** of your codes.

Name of code: FFCASP

Please rank your preferred target PRACE architecture (1=first choice, 2=second choice, ..., x=not suitable)

System	Architecture	Site	Ranking
HP Cray XC40			4
Intel or AMD cluster without GPU			1
Intel or AMD cluster with GPU			2
Intel clusters with Xeon Phi Co-processors (KNC)			3
Other architecture			5
Don't know			x

DECI | FFCASP

FFCASP: A Massively Parallel Crystal Structure Prediction Algorithm

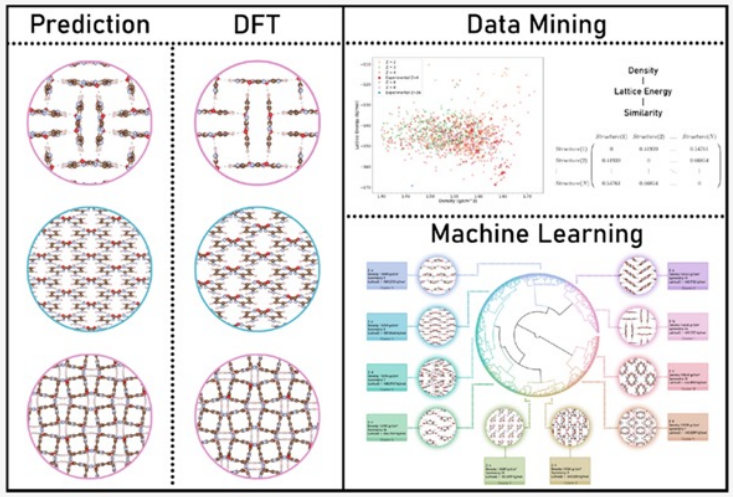
Samet Demir and Adem Tekin*

Cite This: *J. Chem. Theory Comput.* 2021, 17, 2586–2598

Read Online

ACCESS | Metrics & More | Article Recommendations | Supporting Information

ABSTRACT: A new algorithm called Fast and Flexible CrystAl Structure Predictor (FFCASP) was developed to predict the structure of covalent and molecular crystals. FFCASP is massively parallel and able to handle more than 200 atoms in the unit cell (in other terms, it allows global optimization around 100 individual parameters). It uses a global optimizer specialized for Crystal Structure Prediction (CSP) which combines particle swarm and simulated annealing optimizers. Three different molecular crystals, including diverse intermolecular interactions, namely, cytosine, coumarin, and pyrazinamide, have been selected to evaluate the performance of FFCASP. While cytosine polymorphs have been searched by employing two different force fields (a DFT-SAPT based intermolecular potential and generalized amber force field (GAFF)) up to $Z = 16$, only GAFF has been used both in coumarin and pyrazinamide polymorph searches up to $Z = 4$. For these three molecular crystals, FFCASP generated more than 20 000 crystal structures,



DECI | FFCASP – Kovalent kristaller

- $LiMg(BH_4)_3(NH_3)_2$
  - Hydrogen Storage Material
  - FFCASP was successful at finding experimental structure
  - We predicted a lot of good structures (isoenergetic to experimental and phonon calculations show that they are stable)

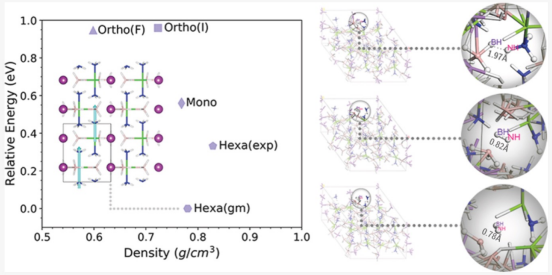
Crystal Structure Prediction and Dehydrogenation Mechanism of $LiMg(BH_4)_3(NH_3)_2$

Gözde İniş Demir, Riccarda Caputo, Samet Demir, and Adem Tekin*

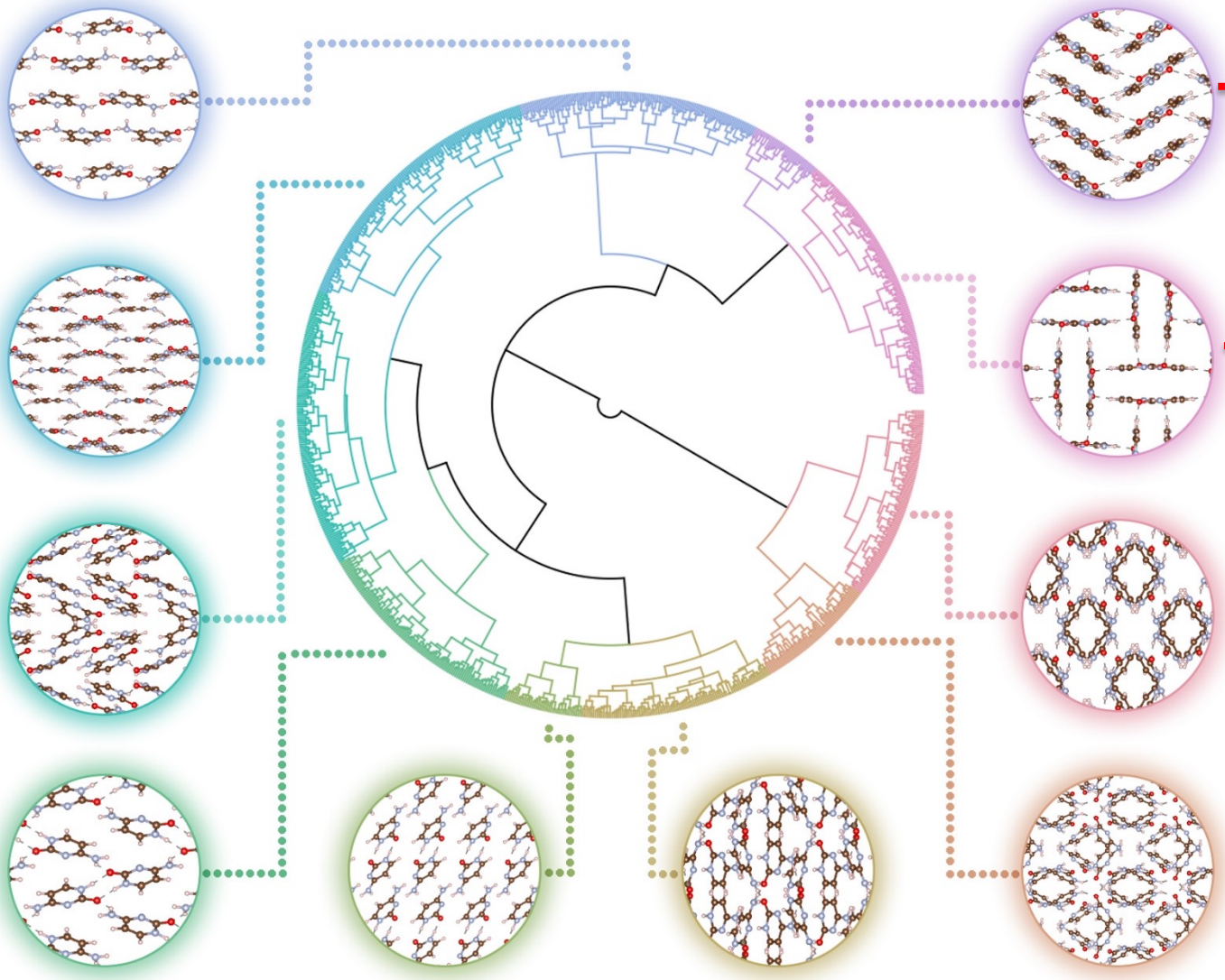
Cite This: *J. Phys. Chem. C* 2021, 125, 10235−10242 Read Online

ACCESS | Metrics & More | Article Recommendations | Supporting Information

ABSTRACT: Dual-cation ammine metal borohydrides are favorable hydrogen storage materials due to their high gravimetric density and relatively low hydrogen release temperature. By combining the Fast and Flexible CrystAl Structure Predictor with density functional theory calculations and Car-Parrinello molecular dynamics, we studied the polymorphism, the lattice stability, and the decomposition mechanism of $LiMg(BH_4)_3(NH_3)_2$ in the temperature range 100−700 K. The onset of $H_2(g)$ formation is found at 400 K through the recombination of the hydrogen atoms from the bond cleavage of B−H and N−H in BH_4 and NH_3 groups. In addition to two hexagonal structures, of which one is the global minimum structure ($P6_3/m$)) and the other corresponds to



DECI | FFCASP – Moleküler kristaller



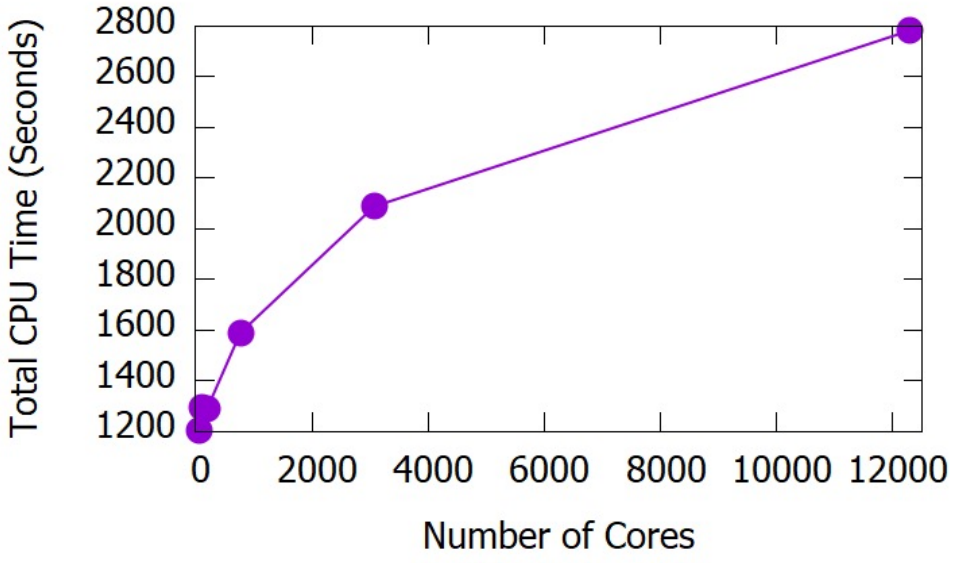
determined in 1964
contains 4 f.u.
orthorhombic $P2_12_12_1$

determined in 2015
contains 16 f.u.
orthorhombic *Pccn*

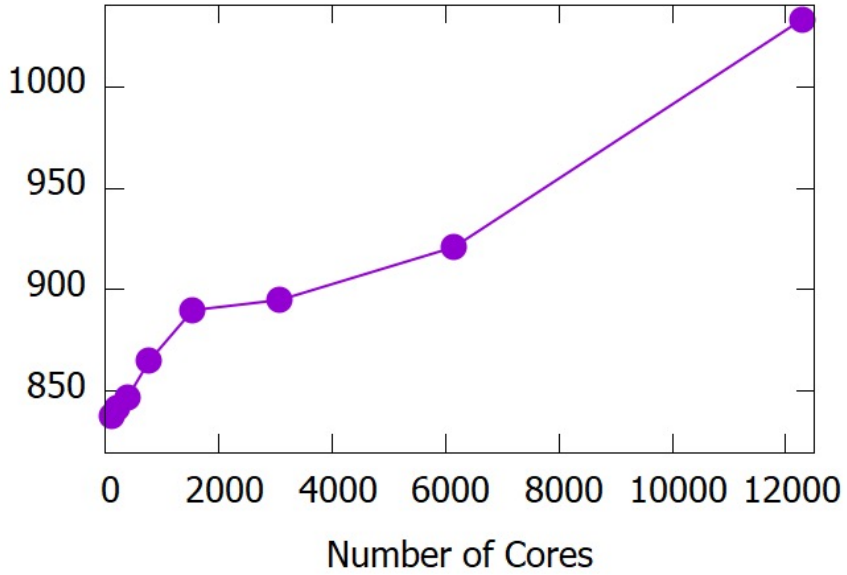
J. Chem. Theory Comput. 2021, 17, 2586–2598

DECI | FFCASP ölçeklenme

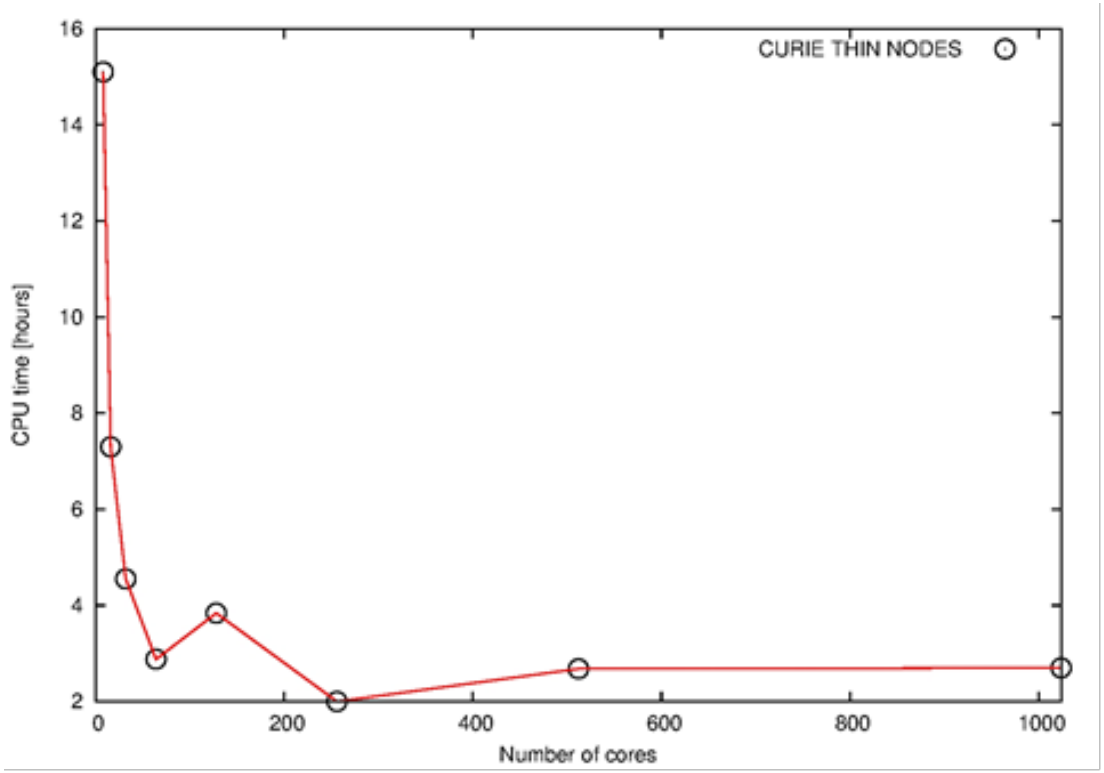
- MareNostrum IV (Barcelona)
- 27th in TOP500 (June 2019)
- Intel Xeon Platinum 8160 24C at 2.1 GHz
- Intel Omni-Path
- No random seed
- 3 predictions



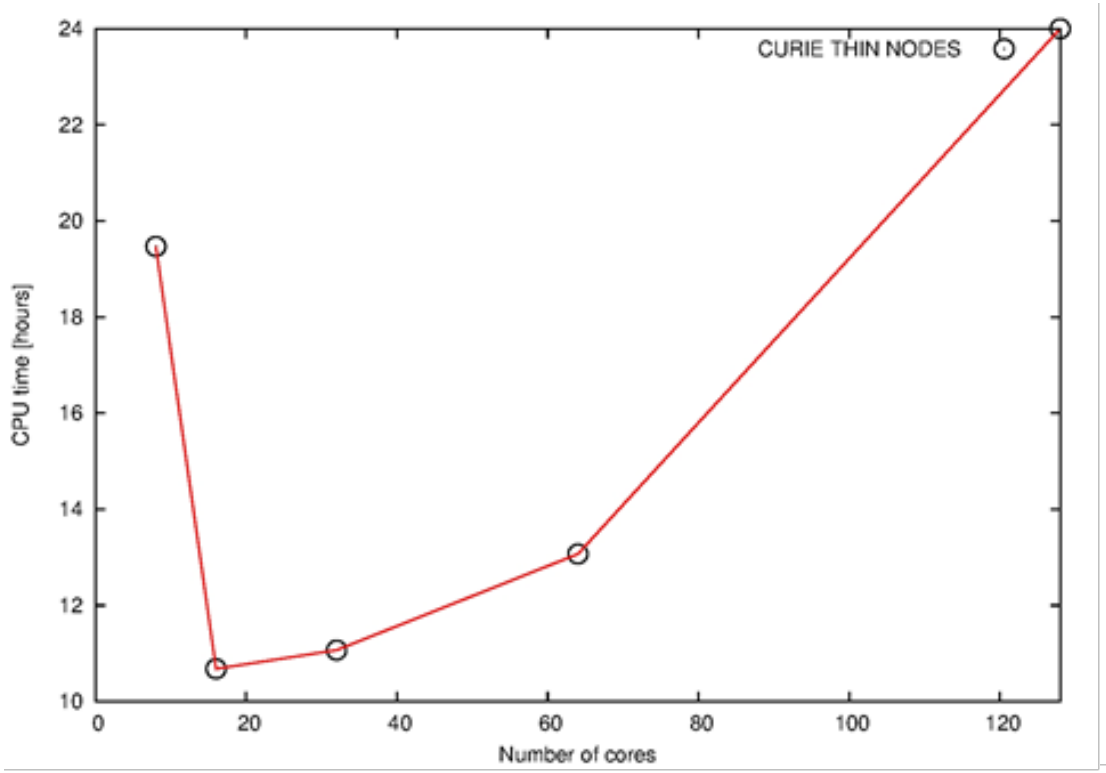
- Hazel Hen (Stuttgart)
- 34th in TOP500 (June 2019)
- Intel Xeon E5-2680v3 12C 2.5GHz
- Aries interconnect
- No random seed
- 2 predictions

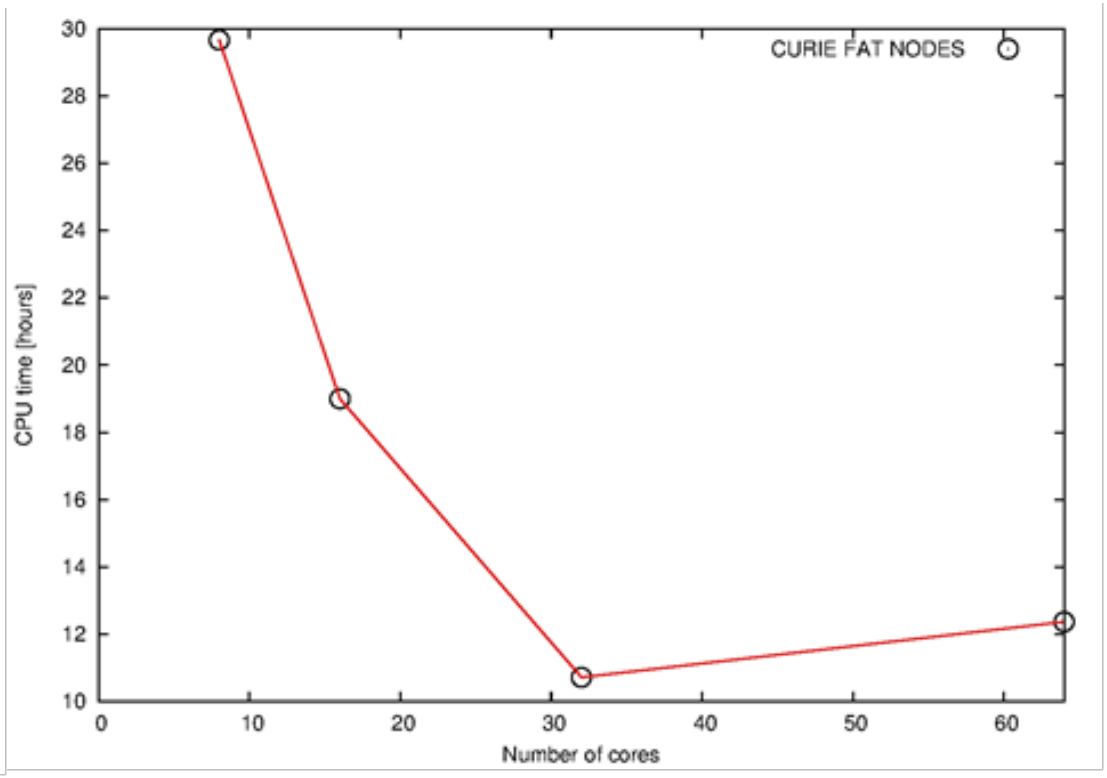


DECI | Quantum Espresso (Katı hal)



DECI | Turbomole (Kuantum Kimya)





Please give the motivation for your preferences above:

FFCASP (Fast & Flexible Crystal Structure Predictor) is capable of using the AVX512 feature of Intel architectures. We gain at least %20 percent speed up in the total run time with AVX supported recent Intel Skylake machines.

Total core-hours based on first preference of architecture	6,000,000
Please give a description of the machine on which the estimate is based (e.g. processor type/speed, web link if available)	
The Kay machine at ICHEC (https://www.ichec.ie/about/infrastructure/kay). Based on test computations on Kay machine using Intel Xeon Gold 6148 (40 cores): 1 FFCASP job requires in between 0.1 to 8 hours with 40 cores. Computation time increases with system size.	
Select all the machines on which the code has been ported	☑ **HP Cray XC40** ☑ **Intel or AMD cluster without GPU** ☑ **Intel or AMD cluster with GPU** ☑ **Intel clusters with Xeon Phi Co-processors (KNC)** ☐ **Other architecture** ☐ **Don't know** **Details:** Intel Skylake is preferable
Please list the details of your regular jobs. Short description (E.g. Structural Optimisation simulations running on VASP, multi-scale simulations running on LAMMPS, turbulence models simulations running on ANSYS Fluent, etc.):	

Number of runs:	20,000
Number of steps per run:	1
Number of hours per step:	8
Number of cores:	40
Minimum time between checkpoints/job restarts (All batch systems put a limit on the duration of jobs. It is important to know if the minimum time between checkpoints is greater than 24 hours):	1
Maximum memory required per core (note this is per core not node) (GB):	1
Number of core hours:	6,000,000
Minimum core hours if hours need to be reduced:	4,000,000

What applications and/or libraries does this code require

Python, numpy, scipy,BLAS, LAPACK, FFT, MPI libraries, C and Fortran compilers are required.

How is your application parallelized (MPI, OpenMP, Hybrid etc.). If GPU, state whether Cuda/OpenCL.

FFCASP is only parallelized with MPI.

Please check the box if this code I/O intensive? ☑

If checked, please describe your strategy concerning I/O (for example usage of I/O libraries, MPI I/O, NetCDF, HDF5 or other approaches):

This project is not IO intensive.

Other requirements (e.g. data transfer tools, workflow tools, other middleware requirements, dependence on a specific member of local/external staff, funding stream, 3rd party software, outcomes of other project, etc):

The project does not require anything further.

Overall data requirements

In this section, we are interested in the overall data requirements for your project as a whole. Please provide the following information.

What is the amount of data to be transferred to the target platforms before production runs can start (Gbytes):	1
What is the amount of data to be transferred from the target platform after all production runs are finished (Gbytes):	200
How much disk space do we need to reserve for your project at the DECI site (Tbyte)? Note larger requests for archive or active data repositories should be indicated below in the ICEI section.	2
Please check the box if it is possible to start transferring data before all production runs are finished?	☐

Where will the data eventually be stored? (HPC facility, local storage at university, institute):

The data will be locally stored in Informatics Institute.

If any planned runs require extensive amounts of memory, hard disk space, etc., please provide details on how the project (in terms of CPU hours) may be split across multiple platforms.

In particular, FFCASP does not require high amount of memory and disk space. However, Quantum Espresso calculations including larger unitcells might be required extensive amounts of memory and hard disks. In such a case, by tuning the computational setup, calculations may fit to the standard compute nodes. If this is not the case, these kind jobs might be run on fat nodes.

Enabling work for the project

For all codes, for which you request enabling support describe what work has already been done to develop the codes

This should include the following: Describing the main algorithms, how they have been implemented and parallelized, and their main performance bottlenecks and the solutions to the performance issues you have considered. Please provide the name and version of all codes to be used in the project.

For each code that needs to be optimized, please provide the details listed below :

1. **Name and version ;**
2. **Webpage and other references ;**
3. **Licensing model ;**
4. **Contact information of the code developers ;**
5. **Your relationship to the code (developer, collaborator to main developers, end user, etc.).**

There is no need for enabling support for both FFCASP and Quantum Espresso. FFCASP is developed in our research group and it can easily be installed to any HPC machine. Quantum Espresso is one of the most popular and open-access periodic Density Functional Theory code which is already installed on majority of HPC machines.

Readiness for production runs

Please note that only limited enabling effort is available from DECI. Please describe what enabling work will need to be completed before production runs can begin.

There is no need for enabling support for both FFCASP and Quantum Espresso.

Routes for dissemination

Discuss the routes that you will use for dissemination of the project and for any appropriate knowledge transfer. This should include any resources that you will be using to support this. (Maximum 500 words)

Dissemination will be via scientific papers. In addition, project outcomes will also be disseminated via national and international conferences.

Confidentiality

Is any part of the project covered by confidentiality? : No
If YES, please give the reasons for confidentiality:

Recent bibliographic references that are relevant to the project

Other support

Do you have any other support for this application e.g. from your national funding council, the EC or international collaborations?

Please give details of this below:

Currently, there is no financial support this project. However, due to the importance of the project subject, a proposal will be prepared and submitted to national funding agency.

DECI | aldığımız destekler

- DeCI-15: COSHOIP isimli hesaplamalı tarama projemiz 2.5 milyon CPU saatle ARCHER makinası (Birleşik Krallık Ulusal Hesaplama Merkezi) kullanılmak üzere desteklendi
- DeCI-16: 2DCSP isimli iki-boyutlu sistemlerin kristal yapı tahminin yapıldığı projemiz yaklaşık 9 milyon CPU saatle Cartesius & Snellius (Hollanda Ulusal Hesaplama Merkezi) makinalarında kullanmak üzerine desteklendi

TEŞEKKÜRLER