密度汎関数理論の最近の発展

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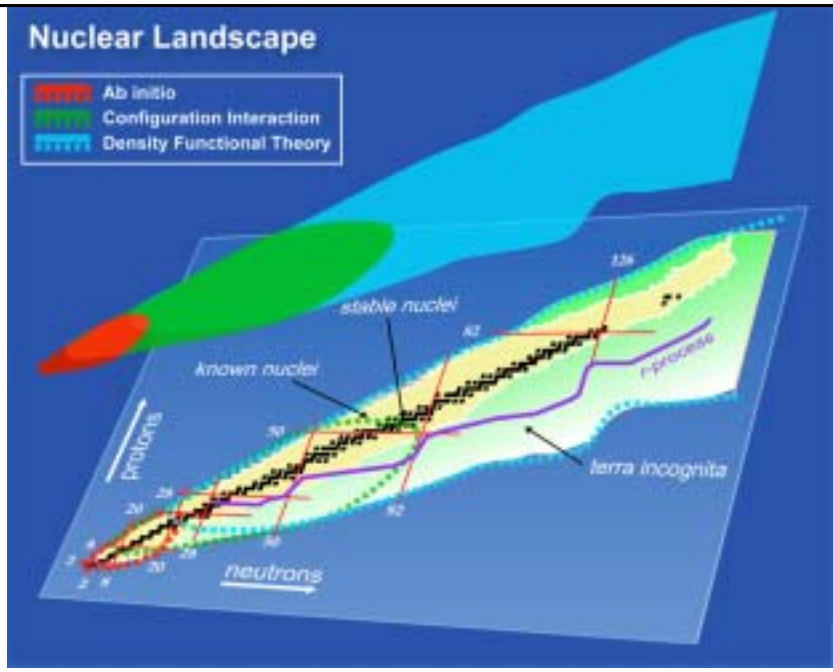
•海外の最近の発展

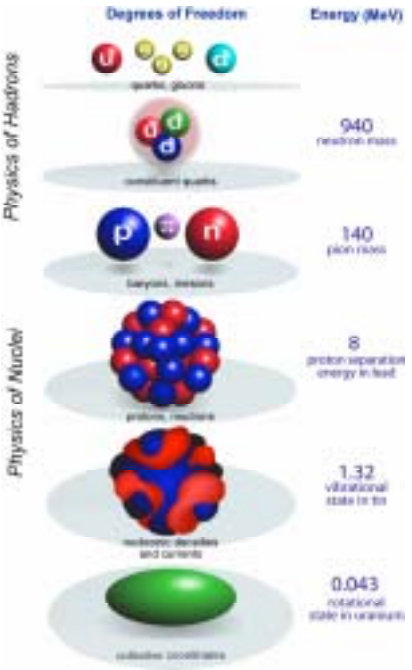
•我々の最近の結果

•GDR, Pygmy GDR

2009.7.27-29 **宇宙核物理連絡協議会主催 第2回研究戦略ワークショップ**



全核種を対象に研究できる。“原理的”にはexactたり得る。

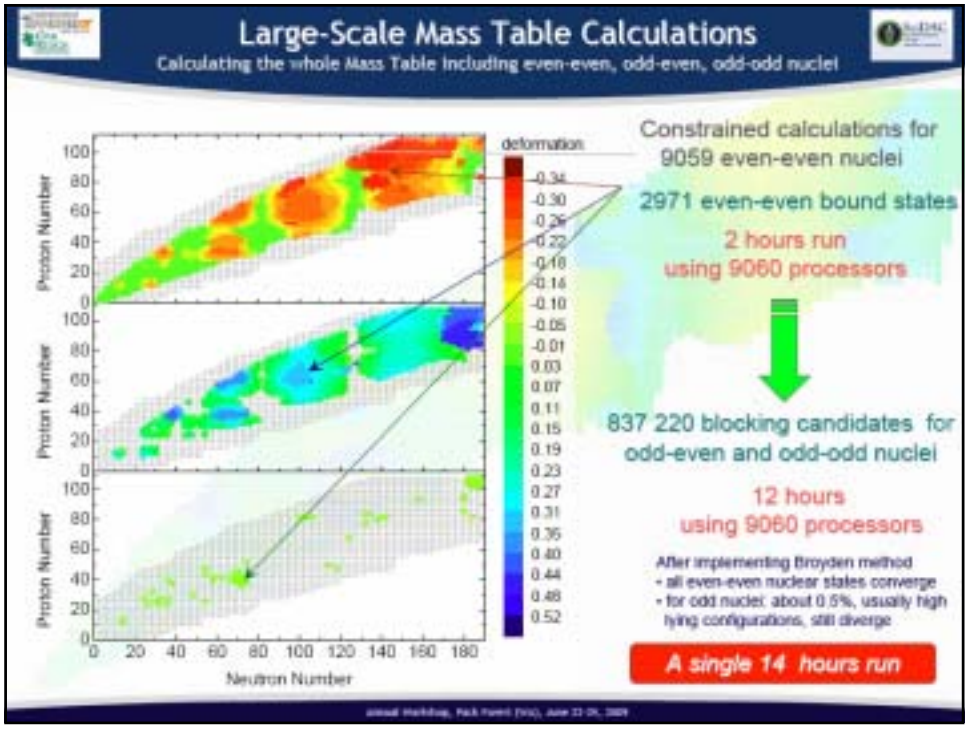


密度汎関数理論によって記述しようとするエネルギー範囲

GeV ~ keV

原子核ＤＦＴの最近の発展

- **アメリカ** SciDAC **プロジェクト** UNEDF (Universal Nuclear Energy Density Functional)
  - **基底状態の汎用コード**（”HFBTHO” by Stoitsov）
  - http://unedf.org
  - http://massexplorer.org
  - **時間依存版コード（ＴＤＨＦＢ）開発**
- Gogny-HFB (Bruyères-le-Châtel group)
  - 5-dim. Collective Schroediner equation



基底状態に関する計算

- 系統的計算が汎用的に可能に
  - –Ab-inito計算の助けを借りて、Energy functionalを最適化（目標：質量誤差500 keV以下）
- 偶核の計算
  - –（１００テラ級のＰＣクラスターがあれば）、１，２時間で偶偶核全種の結果を出せる汎用コード
- 奇核の計算
  - –Odd-even mass differenceは実験をよく再現 (Pairing channel の functional には依存)
  - –Filling approx.の正当性
  - –スピン・パリティを正確に予言することは未だ困難な課題

励起状態に関する計算

Collective Hamiltonian in 5-dim. quadrupole collective coordinates constructed by the constrained HFB calculation

$$\hat{H}_{coll} = \frac{\hbar^2}{2}\sum_{k=1}^{3}\frac{\hat{I}_k^{\,2}}{J_k} - \frac{\hbar^2}{2}\sum_{\mathrm{m,n=0\ and\ 2}} D^{-1/2}\frac{\partial}{\partial a_m}D^{1/2}\left(B_{mn}\right)^{-1}\frac{\partial}{\partial a_n} + V(a_0,a_2) - \Delta V(a_0,a_2)$$

$a_0 = \beta\cos\gamma \qquad a_2 = \beta\sin\gamma$

$J_k(a_0, a_2)$: moment of inertia → « Thouless-Valatin »

$B_{mn}(a_0, a_2)$: collective mass (vibration) → « Cranking »

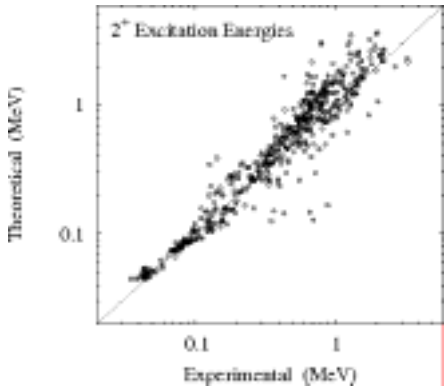
$D(a_0, a_2)$: metric $\qquad D(a_0,a_2) = \prod_{k=1,3} J_k(a_0,a_2)\,\det(B)$

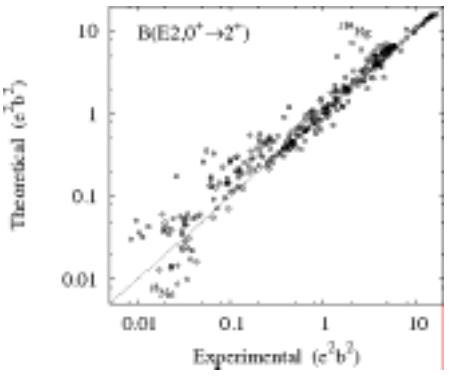
$V(a_0,a_2) = \left\langle \Phi_q \middle| \hat{H} \middle| \Phi_q \right\rangle$

$\Delta V(a_0,a_2) = \mathrm{ZPE} \quad (\mathrm{rot.}+\mathrm{vib.})$ $\qquad ZPE_{pot}$ neglected

Delaroche et al, 2009 Pack Forest Meeting

Properties of the first 2^+ levels





Gogny-HFB + GOA

G.F. Bertsch et al., PRL 99, 032502 (2007)

Time-dependent density functional theory

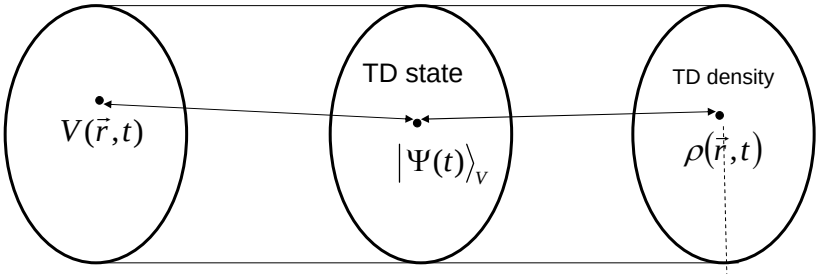
(3D lattice simulation for Skyrme functionals)

Mostly the functional is local in density
→Appropriate for coordinate-space representation

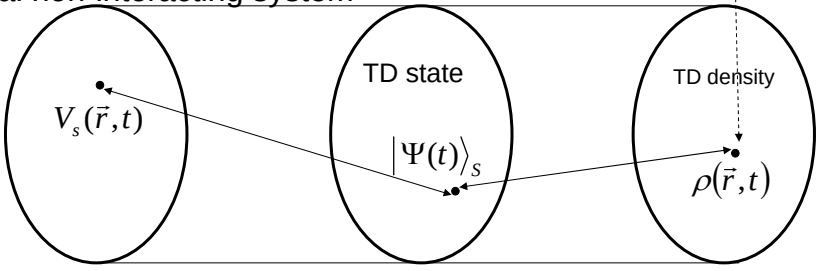
Kinetic energy, current densities, etc. are estimated with the finite difference method

Time-dependen Kohn-Sham Scheme

Real interacting system



Virtual non-interacting system



Time-dependent Kohn-Sham theory

Assuming non-interacting v-representability $\rho(\vec{r},t)=\sum_{i=1}^{N}\left|\phi_i(\vec{r},t)\right|^2$

Time-dependent Kohn-Sham (TDKS) equation

$$i\frac{\partial}{\partial t}\phi_i(\mathbf{r},t)=\left(-\frac{\hbar^2}{2m}\nabla^2+v_s[\rho](\mathbf{r},t)\right)\phi_i(\mathbf{r},t)$$

$$v_s[\rho](\mathbf{r},t)=\frac{\delta\bar{S}[\rho]}{\delta\rho(\mathbf{r},t)}$$

$$\bar{S}[\rho]\equiv S[\rho]-\int_{t_0}^{t_1}\left\langle\Phi_D[\rho](t)\left|i\frac{\partial}{\partial t}-T\right|\Phi_D[\rho](t)\right\rangle$$

Solving the TDKS equation, in principle, we can obtain the exact time evolution of many-body systems.

The functional depends on $\boldsymbol{\rho}(\boldsymbol{r},t)$ and the initial state $\boldsymbol{\Psi}_0$.

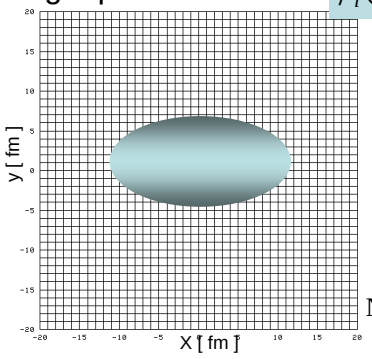
Skyrme TDDFT in real space

Time-dependent Kohn-Sham equation $-i\tilde{\eta}(r)$

$$i\frac{\partial}{\partial t}\psi_i(\mathbf{r}\sigma\tau,t)=\left(h_{\mathrm{KS}}[\rho,\tau,\mathbf{j},\mathbf{s},\vec{\mathbf{J}}](t)+V_{\mathrm{ext}}(t)\right)\psi_i(\mathbf{r}\sigma\tau,t)$$

3D space is discretized in lattice

Single-particle orbital: $\varphi_i(\mathbf{r},t)=\{\varphi_i(\mathbf{r}_k,t_n)\}_{k=1,\cdots Mr}^{n=1,\cdots Mt},\quad i=1,\cdots,N$



N: Number of particles

Mr: Number of mesh points

Mt: Number of time slices

Spatial mesh size is about 1 fm.

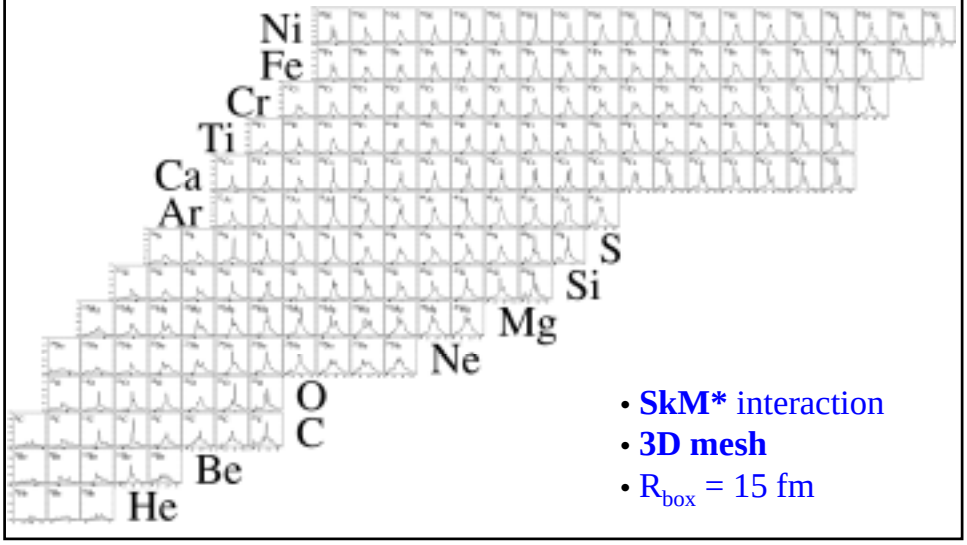
Time step is about 0.2 fm/c

Nakatsukasa, Yabana, Phys. Rev. C71 (2005) 024301

Electric dipole responses

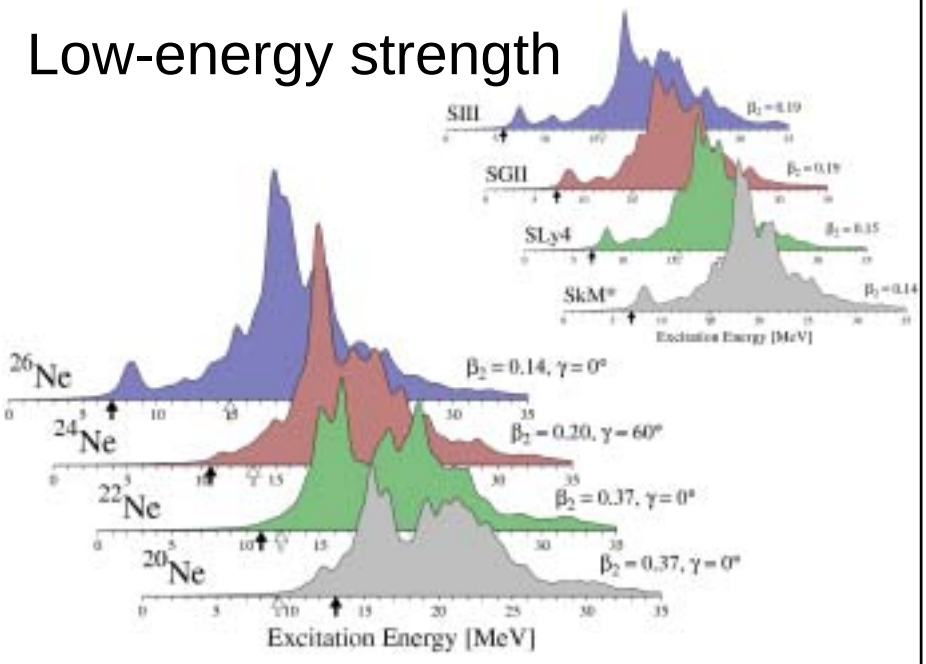
Finite amplitude method to Skyrme-HF+RPA

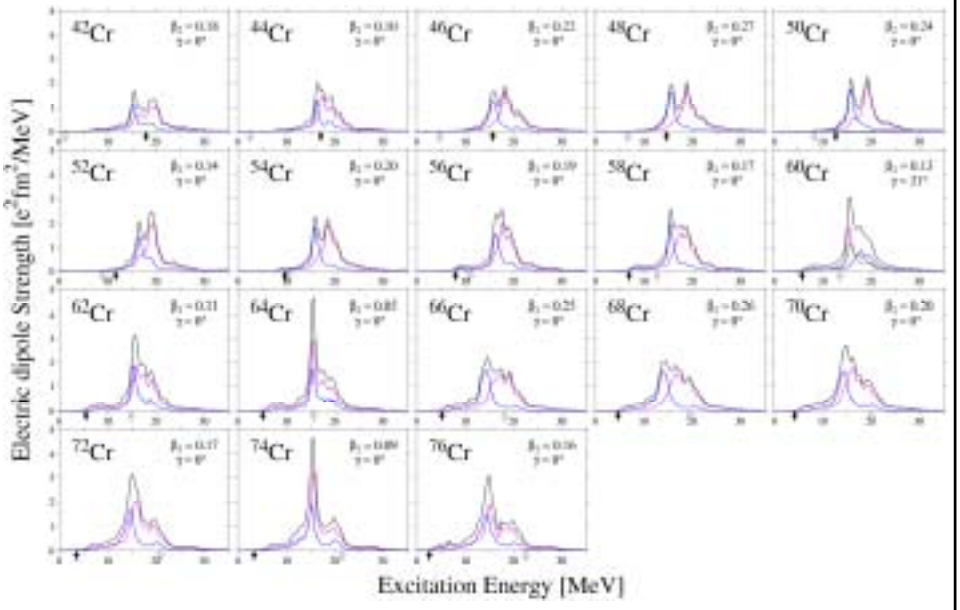
Inakura, Nakatsukasa, Yabana, arXive:0906.5239



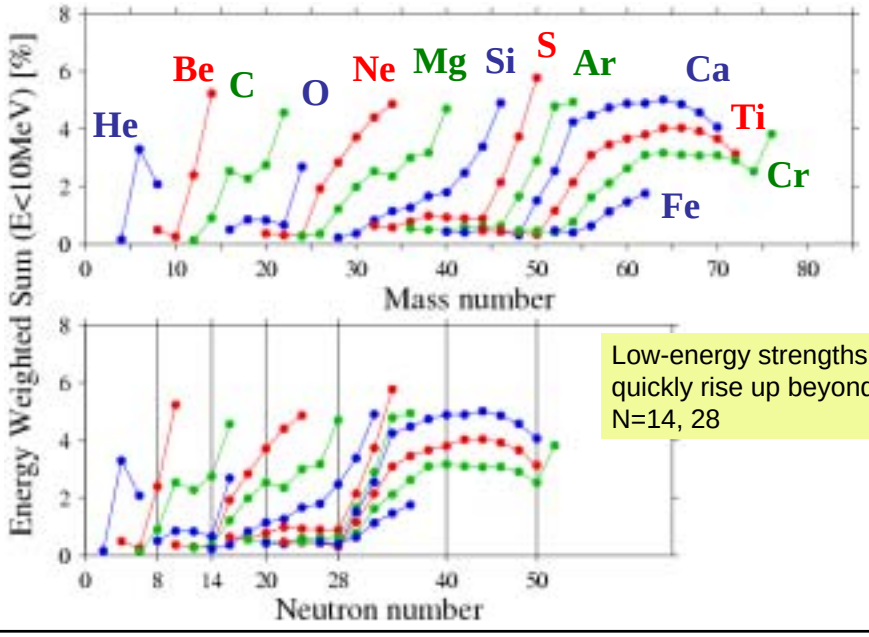
- **SkM*** interaction
- **3D mesh**
- R_{box} = 15 fm

Low-energy strength





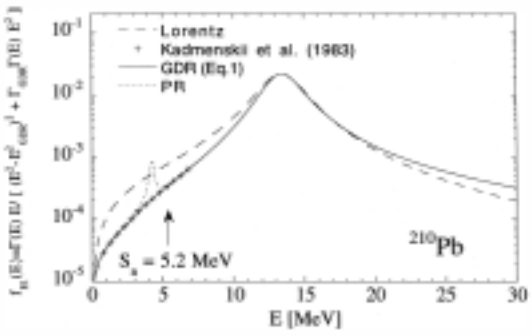
Low-lying strengths

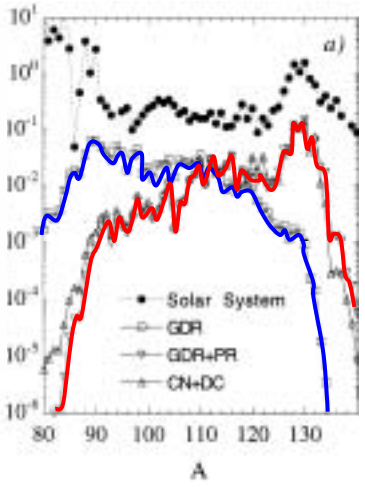


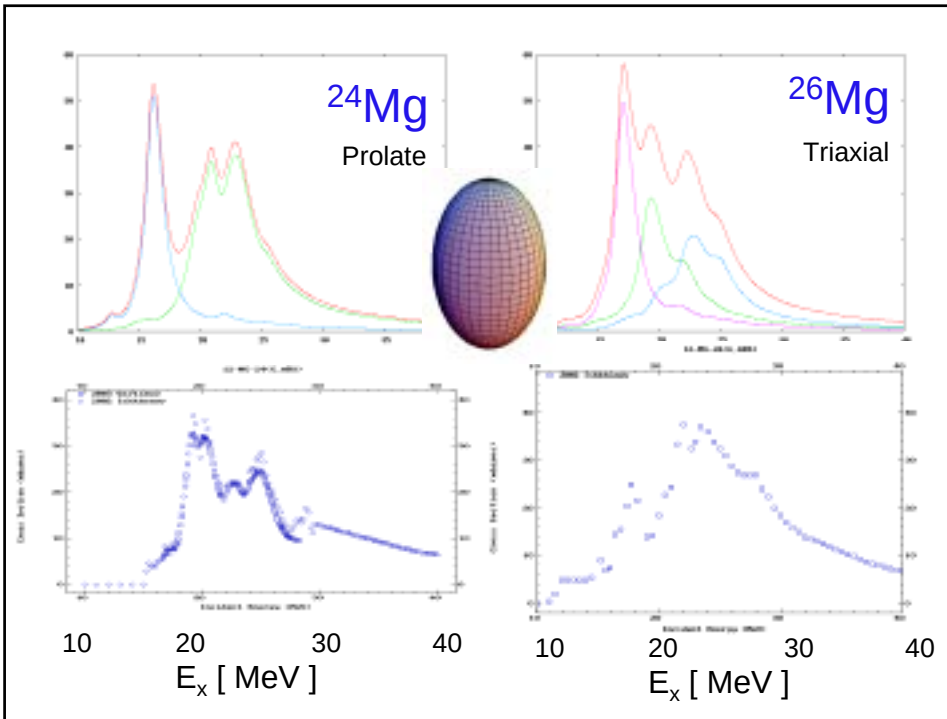
Low-energy strengths quickly rise up beyond N=14, 28

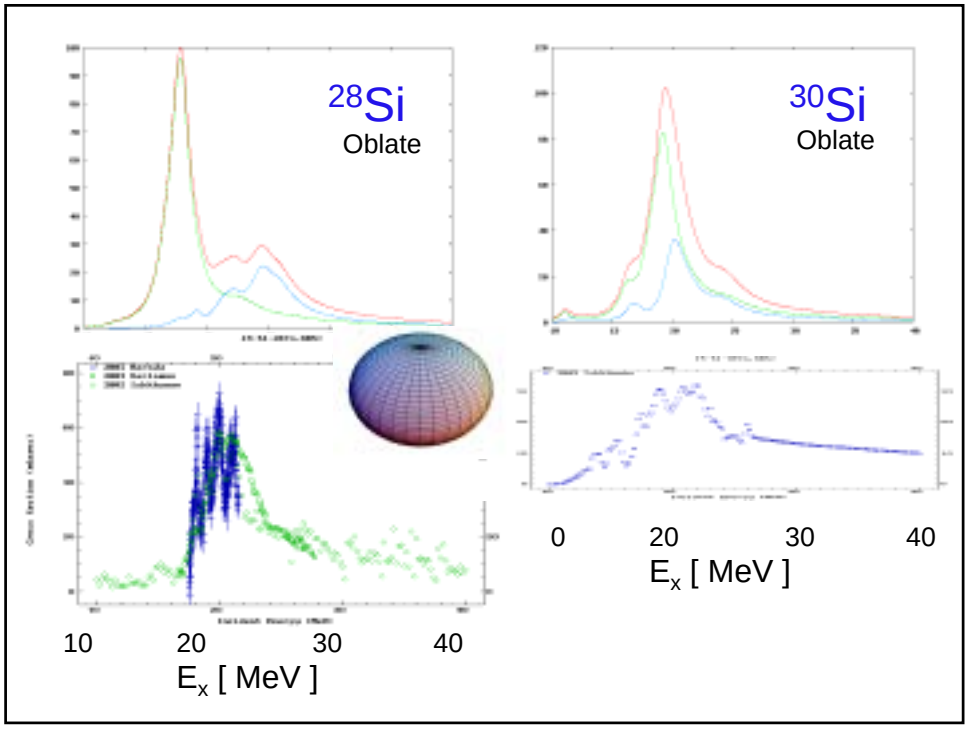
PDR: impact on the r-process

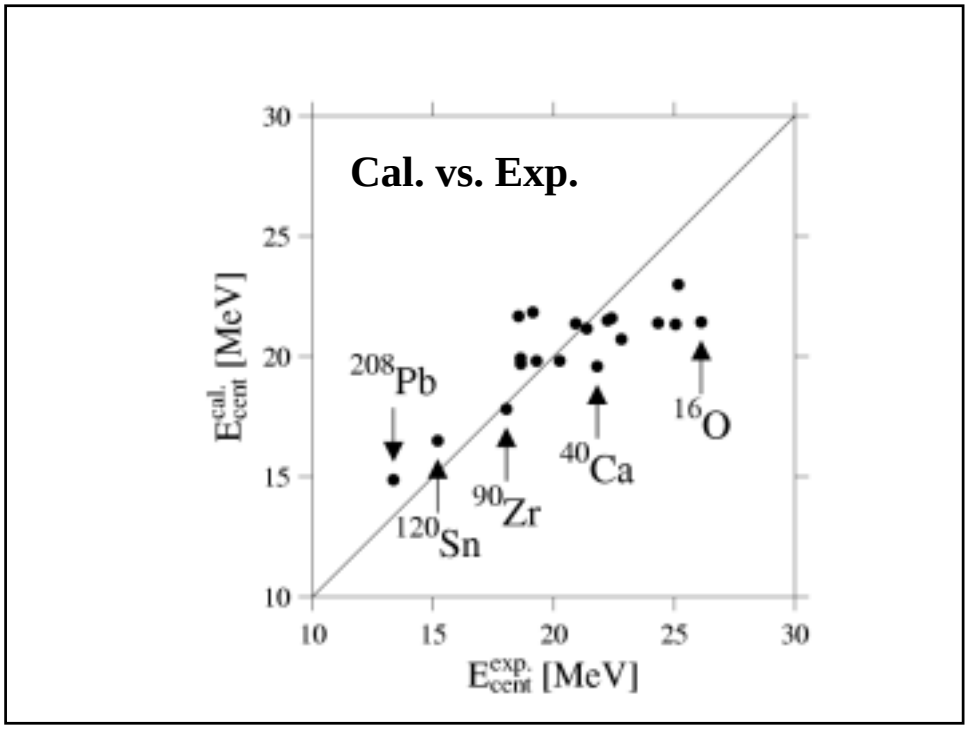
S. Goriely, Phys. Lett. **B436**, 10.



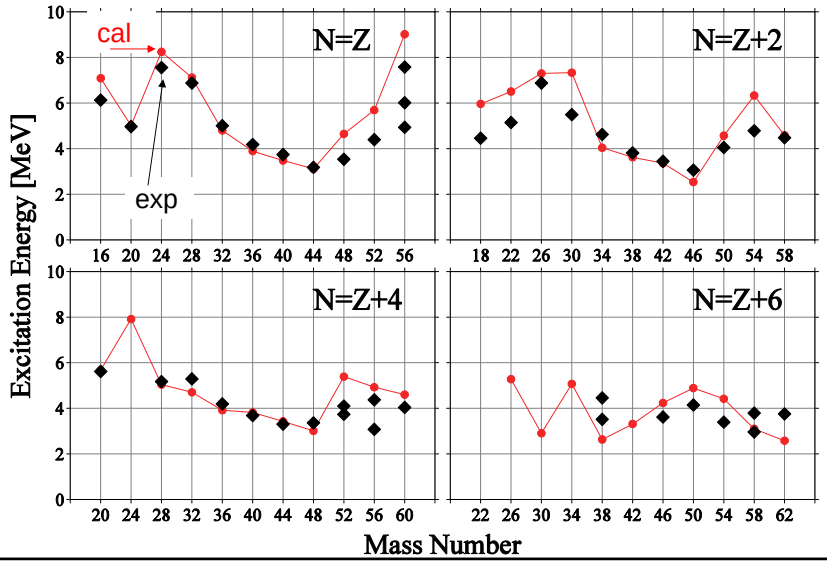





28Si
Oblate
30Si
Oblate
10
20
30
40
Ex [MeV]
0
20
30
40
Ex [MeV]


Cal. vs. Exp.
30
25
20
15
10
10
15
20
25
30
Ecent.cal. [MeV]
Ecent.exp. [MeV]
208Pb
120Sn
90Zr
40Ca
16O

Lowest negative-parity states (SGII functional)



Summary

世界の現状と我々のアプローチ

- 核質量（束縛エネルギー）については、実験との誤差を解消するため、Kohn-Shamスキームでは組み入れられていない相関エネルギーの計算法を開発中
- 効率の高い計算コードの開発
- 励起状態・遷移強度の記述については、ＴＤＤＦＴに基づく記述が発展しており、変形（Q）ＲＰＡコードの開発が進行（Terasaki-Engel, Peru-Goutte,
  - 我々は、実時間法と有限振幅法によるアプローチにより、計算コードを開発 (Inakura, Ebata)
- 調和近似を超えた扱いについても最近発展あり
  - ＴＤＤＦＴに準拠するものとして、断熱型自己無撞着集団座標法に基づくものを開発中 (Hinohara, Sato)