# Electronic structure of superheavy elements and vacuum decay

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with the PNPI group:
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and with
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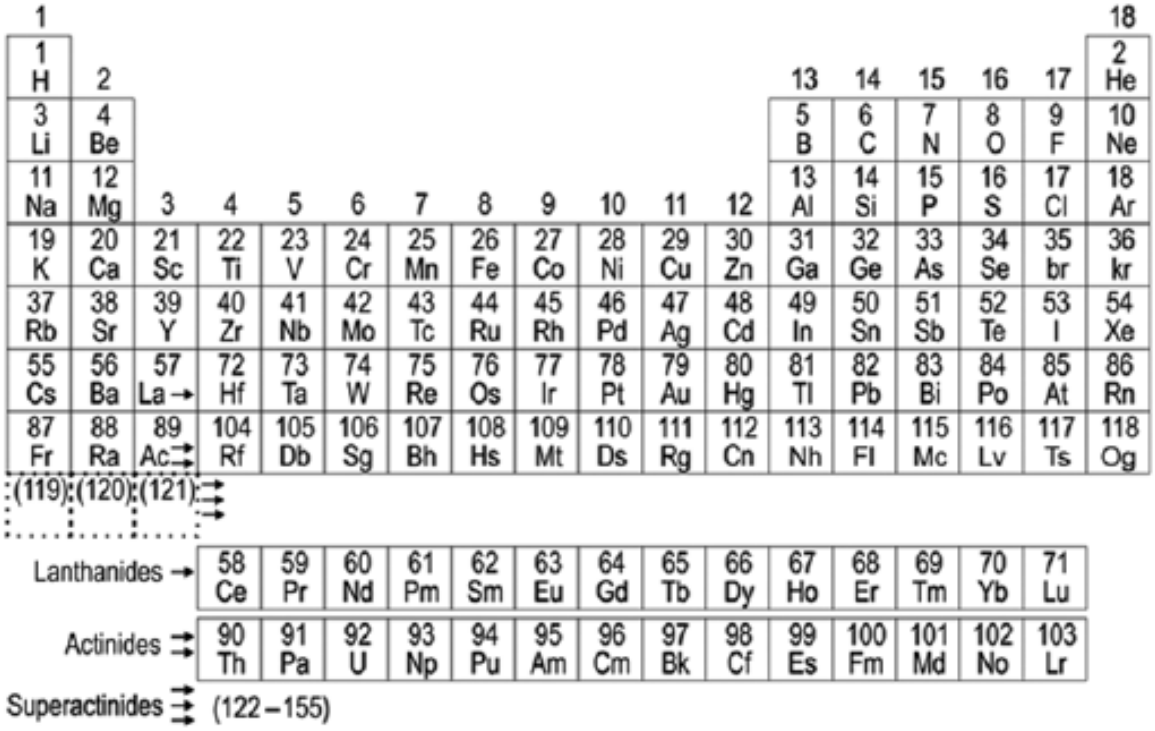
# Outline of the talk

- Introduction
- The work of the SPbSU group on SHE
  - Electronic structure of SHE
  - Chemical properties of SHE
  - Calculations of SHE with quantum algorothms
- QED at supercritical Coulomb field
  - Pair creation in heavy-ion collisions
  - How to observe the vacuum decay
- Conclusion

# Electronic structure of superheavy elements




The table is taken from V. Pershina, Radiochim. Acta 107, 833 (2019).

For the recent prediction in the range $Z = 119 - 172$ see also: *O.R. Smits et al., Nature Reviews Physics, 2023.*

# Electronic structure of superheavy elements

In the last five years we performed the electronic-structure calculations for a number of super-heavy elements (SHE) of the 7th and 8th periods with atomic numbers $110 \leq Z \leq 170$ and their lighter homologous [1-6].

- Ground state electron configurations of superheavy elements (SHE)
- Ionization potentials
- Electron affinities
- One-particle electron density. Root-mean-square radii (RMS) and widths of the electron-density distribution of valence shells
- Electron localization functions (ELF)
- Orbital collapse
- Quantum electrodynamics (QED) corrections ($110 \leq Z \leq 170$)


1. *M.Y. Kaygorodov et al., Proseedings of Science (FFK2019) 036 (2019).*
2. *M.Y. Kaygorodov et al., Phys. Rev. A 104, 012819 (2021).*
3. *I.I. Tupitsyn et al., Optics and Spectroscopy 129, 1038 (2021).*
4. *M.Y. Kaygorodov et al., Phys. Rev. A 105, 062805 (2022).*
5. *I.I. Tupitsyn et al., Optics and Spectroscopy, 130, 1022 (2022).*
6. *A.V. Malyshev et al., Phys. Rev. A 106, 012806 (2022).*
7. *I.M. Savelyev et al., Phys. Rev. A, 107, 042803 (2023).*
8. *I.I. Tupitsyn et al., Phys, Rev. A, 109, 042807 (2024).*

## How Far Does the Periodic Table Go?

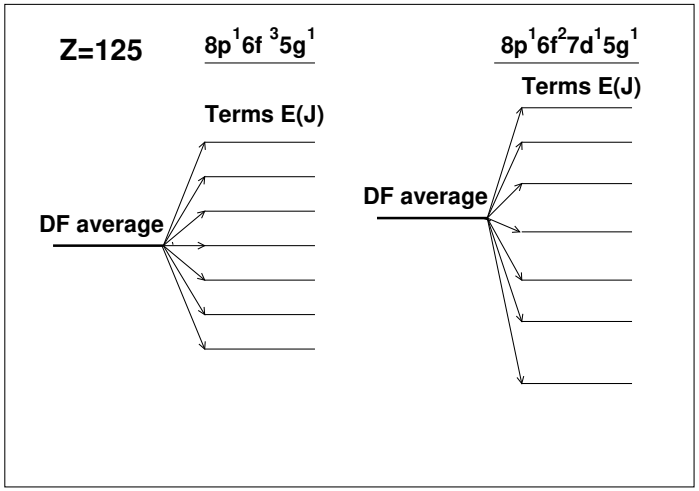
The electronic structure of SHEs is unique in several aspects:

- The concept of the ground configuration for SHEs of the 8th period is no longer well-defined, since sets of relativistic atomic terms of different configurations are overlapping [1].
- Strong relativistic effects cause **contraction of the $s_{1/2}$- and $p_{1/2}$- orbitals**, i.e., the shift of the maximum of the density distribution of these shells to lower values of the radius and an increase in the binding energies of these electrons.
- Spin-orbital splitting of valence p-shells reaches up to about 10 eV for the 7p-orbital in Og (Z=118) and about 75 eV for the 8p-orbital in element with atomic number Z=165.

[1] *I.M. Savelyev et al., Phys. Rev. A, 107, 042803 (2023).*

# Electronic structure of superheavy elements

**How do we define the ground state configuration?**



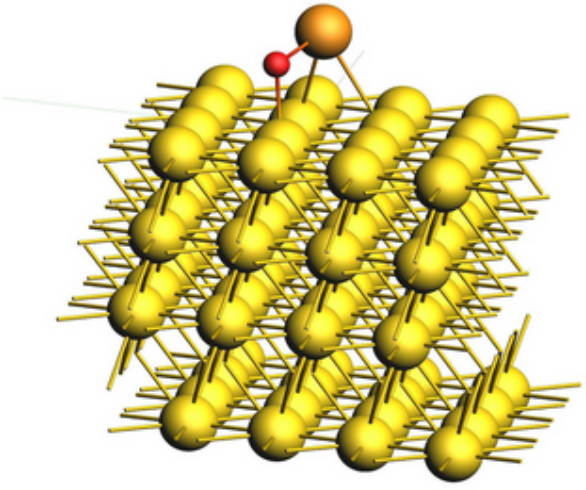

**The ground configuration** is the configuration with the lowest average energy $E^{\rm av}$.
**The ground state level** is the level with the lowest $E(J)$.

**$Z = 125$. The lowest Dirac-Fock energy levels within the configuration average approximation and for the relativistic terms.**

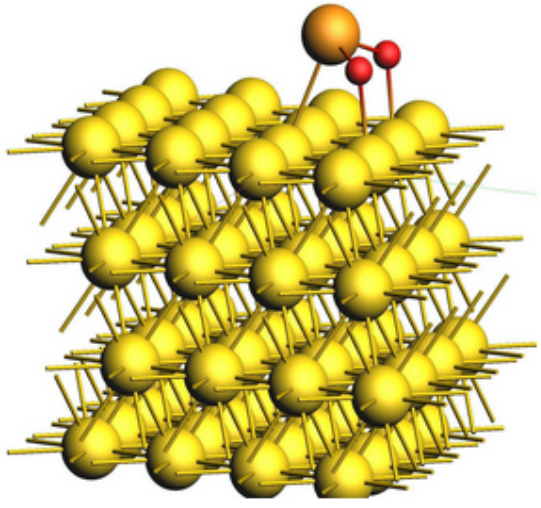
| Configuration | | $E^{\rm av}_{\rm DF}$ [a.u.] | J | $E_{\rm DF}(J)$ [a.u.] |
|---|---|---|---|---|
| $8p^1 6f^3 5g^1$ | $E_1$ | -64627.549597 | 6.5 | -64627.614303 |
| $8p^1 6f^2 7d^1 5g^1$ | $E_2$ | -64627.542119 | 8.5 | -64627.638846 |
| | $\Delta E = E_2 - E_1$ | 0.007478 | | -0.024543 |

*These configurations have different parity and do not mix.*

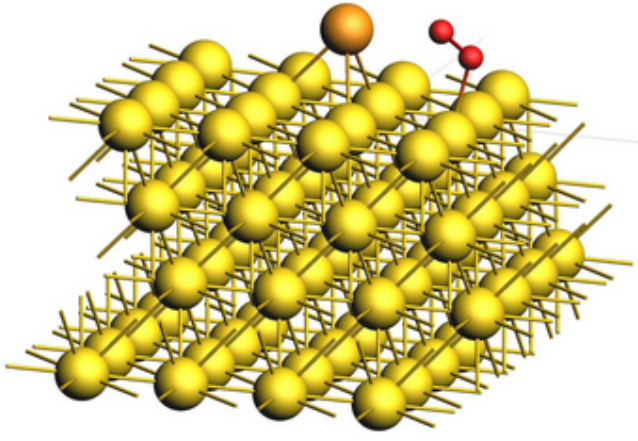
# Adsorption of SHEs and their compounds on Au(111) Surface



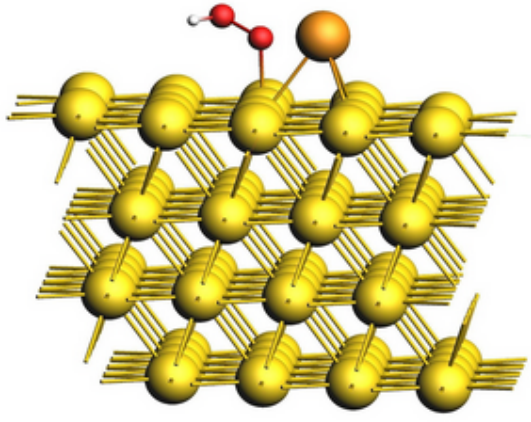
TsO



$TsO_2$



TsOO

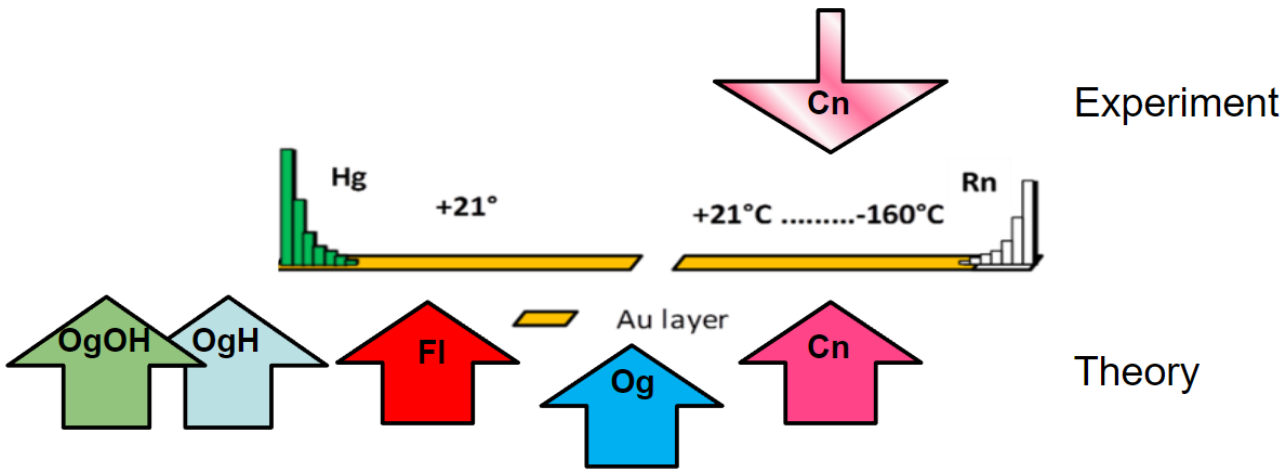


TsO(OH)

# Adsorption energy studies of SHEs and their compounds on Au(111) Surface

Investigated species

- Atoms
  – Hg/Cn, Tl/Nh, Pb/Fl, Bi/Mc, Po/Lv, At/Ts, Rn/Og
- Compounds
  – hydrides BiH/McH, PoH/LvH, AtH/TsH, RnH/OgH
  – oxides AtO/TsO, $AtO_2$/$TsO_2$, AtOO/TsOO
  – oxyhydrides AtOH/TsOH, RnOH/OgOH, AtO(OH)/TsO(OH)




A. Ryzhkov, V. Pershina, M. Iliaš and V. Shabaev, *Phys. Chem. Chem. Phys.*, **25**, 15362 (2023).
A. Ryzhkov, V. Pershina, M. Iliaš, and V. Shabaev, *Phys. Chem. Chem. Phys.*, **26**, 9975 (2023).

# Adsorption of HgO, CnO, and FlO on Teflon surface

$$E_{\mathsf{ads}}(d) = -\frac{3}{16}\frac{\varepsilon-1}{\varepsilon+2}\frac{\alpha_{\mathsf{mol}}}{\left(\frac{1}{\mathsf{IP}_{\mathsf{mol}}}+\frac{1}{\mathsf{IP}_{\mathsf{surf}}}\right)d^3} - \frac{1}{8}\frac{\varepsilon-1}{\varepsilon+2}\frac{\mu^2_{\mathsf{mol}}}{d^3},$$

- Molecular properties – optimal geometry, electrostatic dipole moment, polarizability, and ionization potential – are calculated within fully relativistic coupled cluster and DFT approaches.
- The adsorption energies ($-E_{\mathsf{ads}}$) on the surface of Teflon:
  - For parallel disposition, HgO $>$ CnO $>$ FlO.
  - For perpendicular, HgO $>$ FlO $>$ CnO.

  The obtained values of $-E_{\mathsf{ads}}$ are low so their delivery from the recoil chamber to the chemistry set up should take place.

A. A. Kotov, Y. S. Kozhedub, D. A. Glazov, M. Iliaš, V. Pershina, and V. M. Shabaev, *ChemPhysChem*, **24**, e202200680 (2023).

# Adsorption of AtH/OH, RnH/OH, TsH/OH, and OgH/OH on Teflon surface

- Molecular properties are calculated within DFT approach.
- SHE compounds and their closest lighter homologs indicate substantial differences across all the considered properties.
- The adsorption energies ($-E_{\mathbf{ads}}$) on the surface of Teflon:
  - For parallel disposition, TsH $\gtrsim$ AtH $>$ OgH $\gtrsim$ RnH.
  - For perpendicular, AtH $\lesssim$ TsH $<$ OgH $\lesssim$ RnH.
  - TsOH $>$ AtOH $>$ OgOH $>$ RnOH (the molecules are arranged so the value of $-E_{\mathbf{ads}}$ is maximized.).

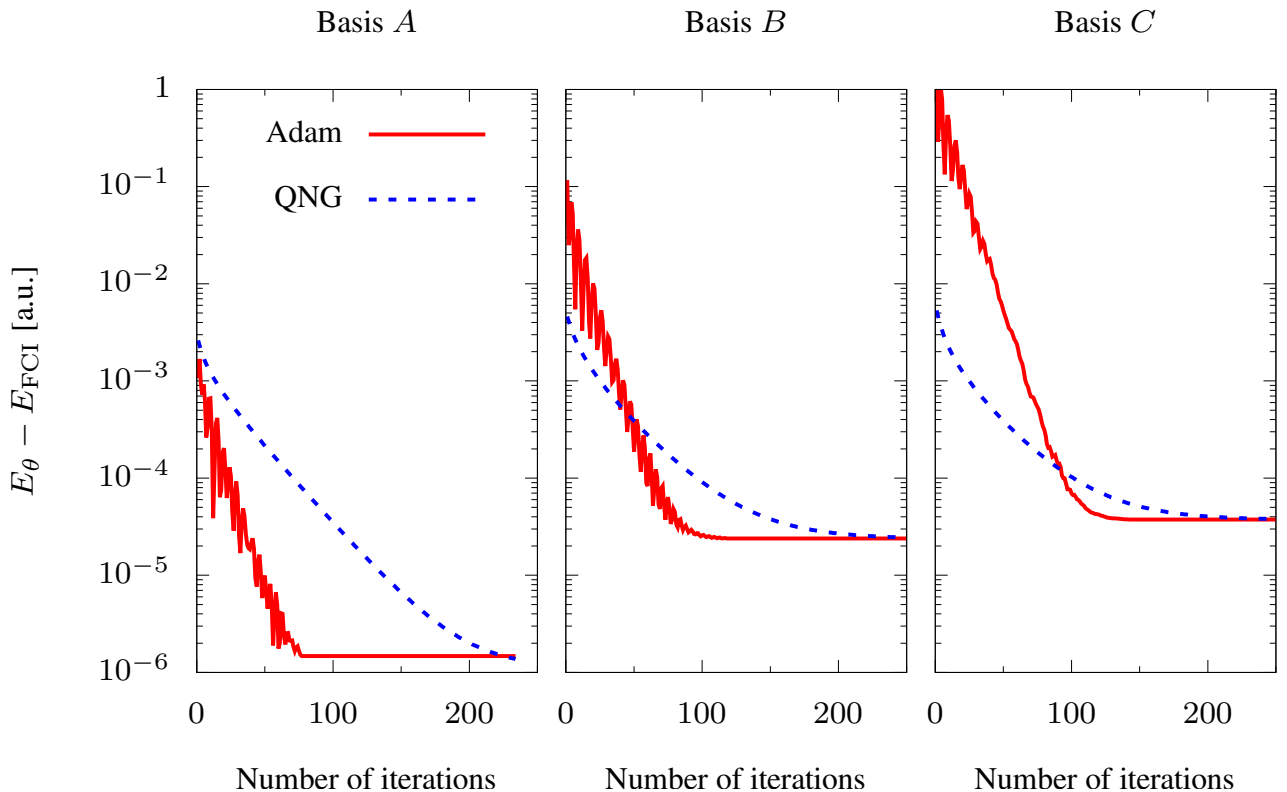
  The obtained values of $-E_{\mathbf{ads}}$ are low, indicating a potential for these molecules to be transported through a Teflon capillary

A. A. Kotov, Y. S. Kozhedub, D. A. Glazov, M. Iliaš, V. Pershina, and V. M. Shabaev, Relativistic calculations of spectroscopic properties of superheavy element compounds with H and OH radicals, in preparation.

# Calculation of the moscovium ($Z = 115$) ground-state energy using quantum algorithms

Quantum algorithms:

- Iterative Phase Estimation algorithm (IPEA)
- Variational Quantum Eigensolver (VQE)
- VQE was tested up to 15 electrons on 26 orbitals ($\approx$ 500000 Sl. det.)
- Adam and QNG optimizers were used

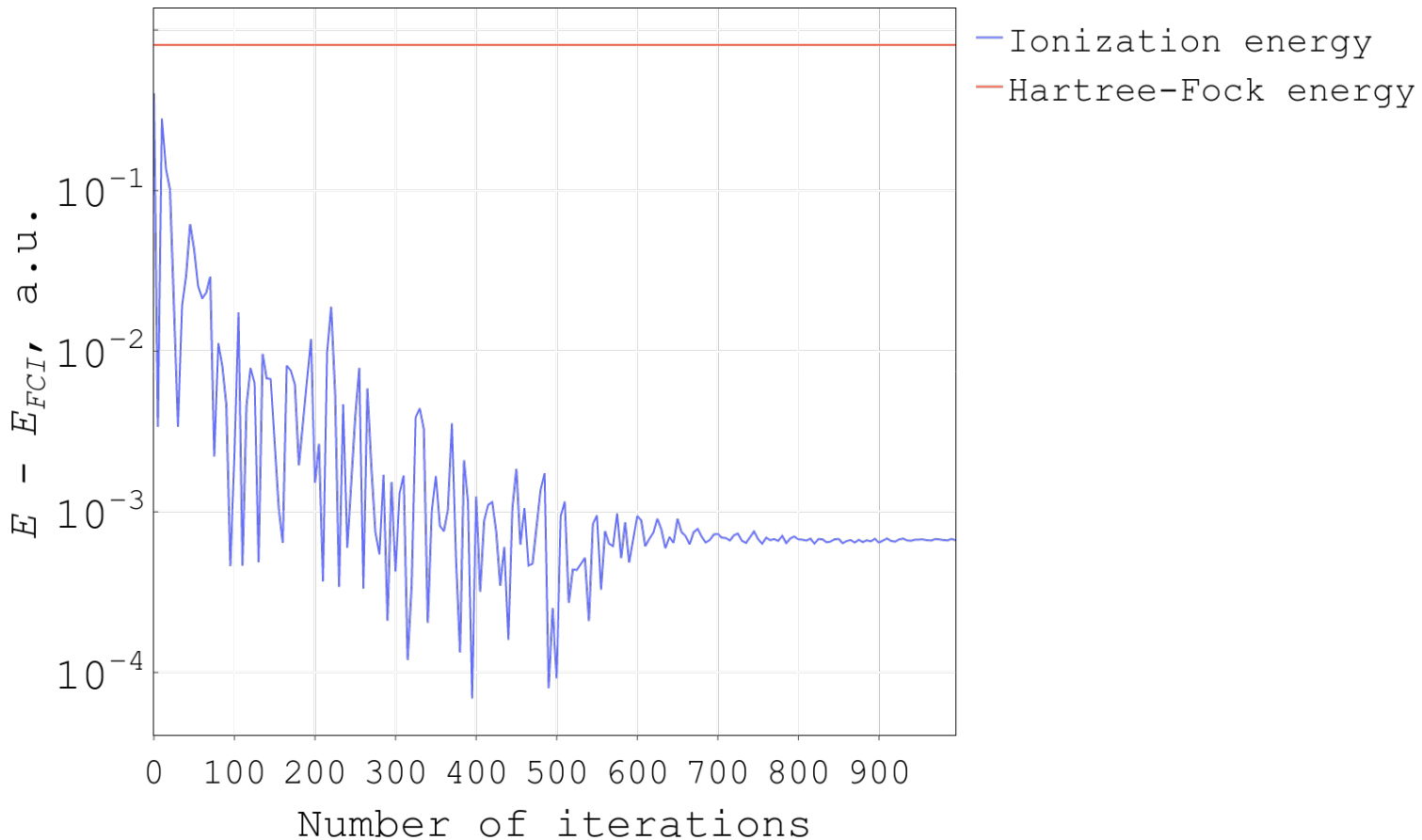



V.A. Zaytsev, M.E. Groshev, I.A. Maltsev, A.V. Durova, V.M. Shabaev, Int. J. Quant. Chem **124**, e27232 (2024).

# New quantum algorithm for direct calculation of ionization energy

Features:

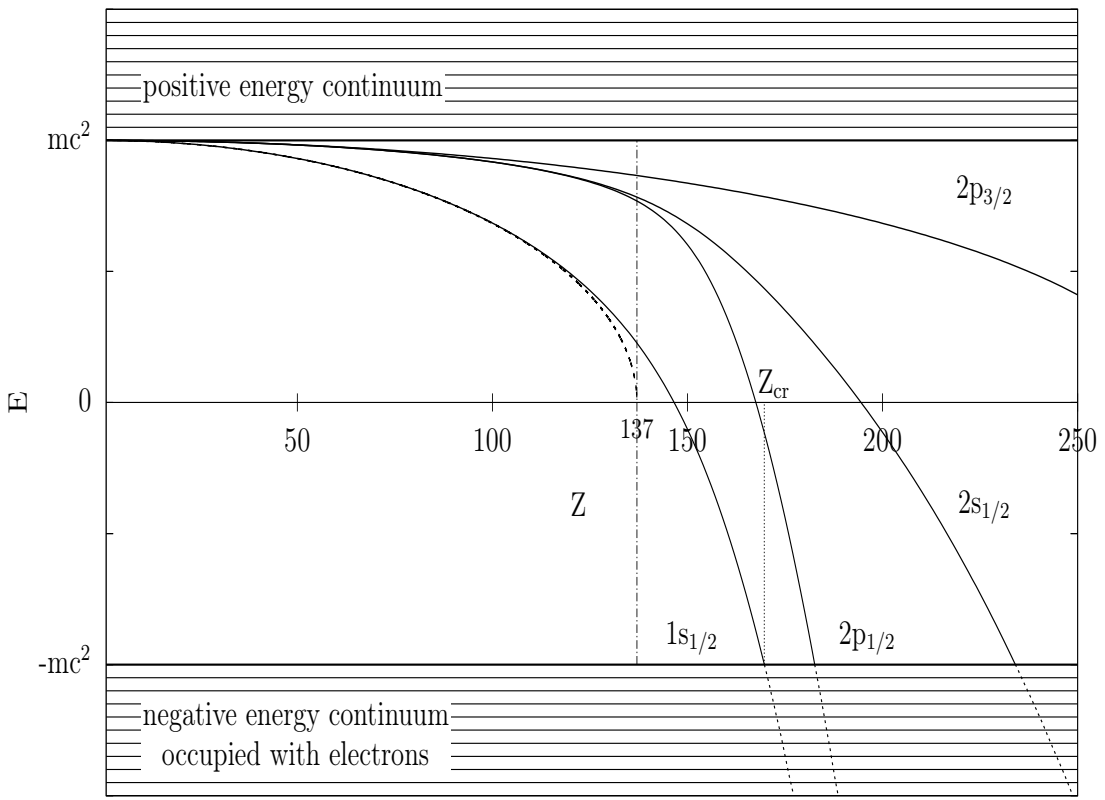
- has a variational nature
- unlike VQE, allows **direct** calculation of ionization energy on a quantum computer




Ionization energy of moscovium atom (UCC ansatz with Adam optimizer)

## Supercritical Coulomb field

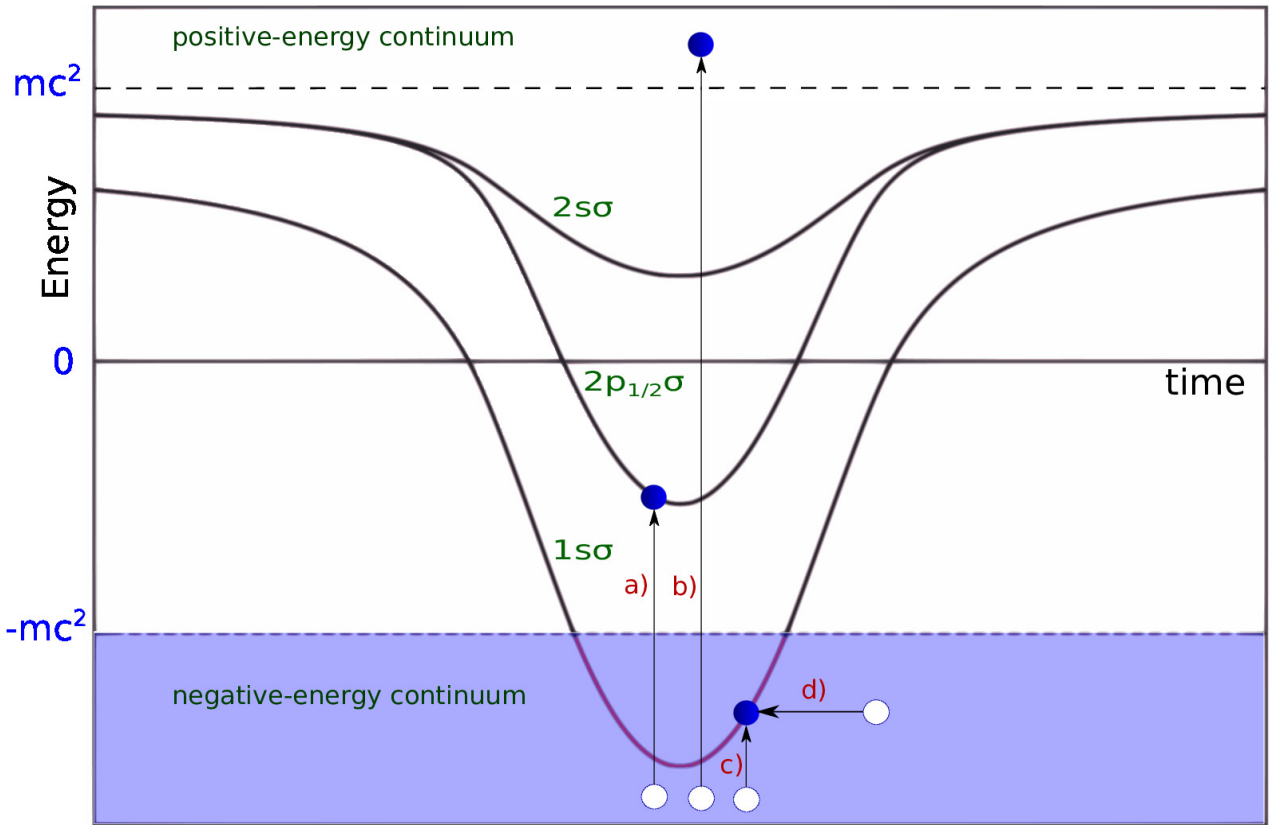
S.S. Gershtein, Ya.B. Zel'dovich, 1969; W. Pieper, W. Greiner, 1969




The $1s$ level dives into the negative-energy continuum at $Z_{\rm crit} \approx 173$.

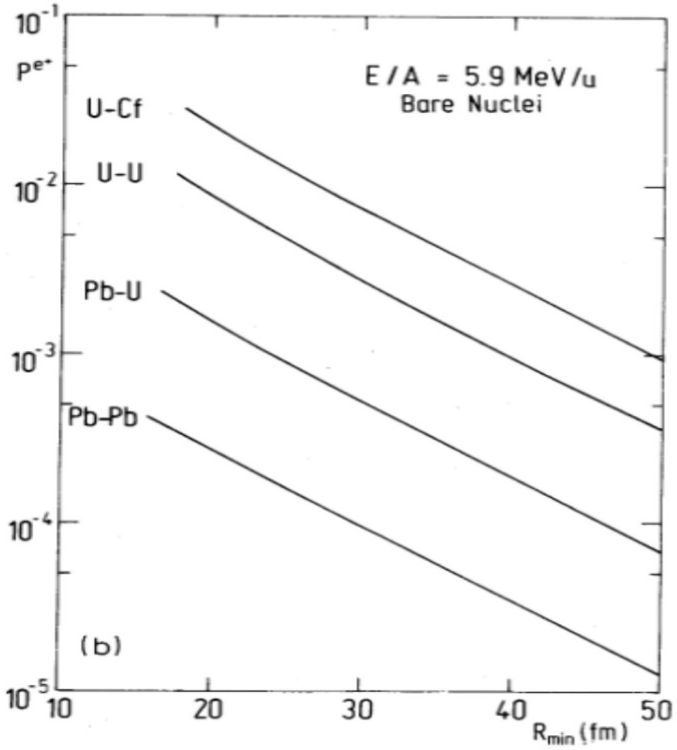
# *Low-energy heavy-ion collisions*

Creation of electron-positron pairs in low-energy heavy-ion collisions, with $Z_1 + Z_2 > 173$




Dynamical mechanism: a),b),c). Spontaneous mechanism (vacuum decay): d). The $1s$ state dives into the negative-energy continuum for about $10^{-21}$ sec.

Positron production probability in 5.9 MeV/u collisions of bare nuclei as a function of distance of closest approach $R_{\min}$
*(J. Reinhardt, B. Müller, and W. Greiner, Phys. Rev. A, 1981).*




Conclusion by Frankfurt's group (2005):The vacuum decay could only be observed in collisions with nuclear sticking, in which the nuclei are bound to each other for some period of time by nuclear forces.

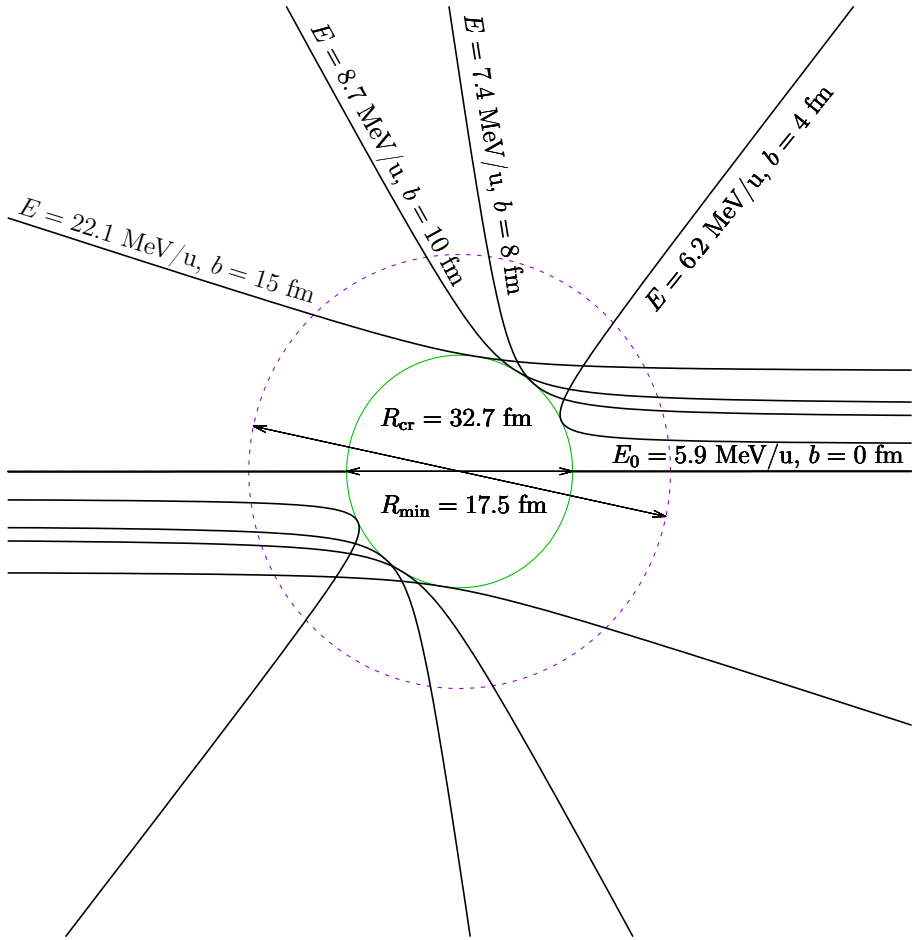
## *Low-energy heavy-ion collisions*

New methods for calculations of quantum dynamics of electron-positron field in low-energy heavy-ion collisions at subcritical and supercritical regimes have been developed:

- *I.I. Tupitsyn, Y.S. Kozhedub, V.M. Shabaev et al., Phys. Rev. A 82, 042701 (2010).*
- *I. I. Tupitsyn, Y. S. Kozhedub, V. M. Shabaev et al., Phys. Rev. A 85, 032712 (2012).*
- *G. B. Deyneka, I. A. Maltsev, I. I. Tupitsyn et al., Russ. J. of Phys. Chem. B 6, 224 (2012).*
- *G. B. Deyneka, I. A. Maltsev, I. I. Tupitsyn et al., Eur. Phys. J. D 67, 258 (2013).*
- *Y.S. Kozhedub, V.M. Shabaev, I.I. Tupitsyn et al., Phys. Rev. A 90, 042709 (2014).*
- *I.A. Maltsev, V.M. Shabaev, I.I. Tupitsyn et al., NIMB, 408, 97 (2017).*
- *R.V. Popov, A.I. Bondarev, Y.S. Kozhedub et al., Eur. Phys. J. D 72, 115 (2018).*
- *I.A. Maltsev, V.M. Shabaev, R.V. Popov et al., Phys. Rev. A 98, 062709 (2018).*

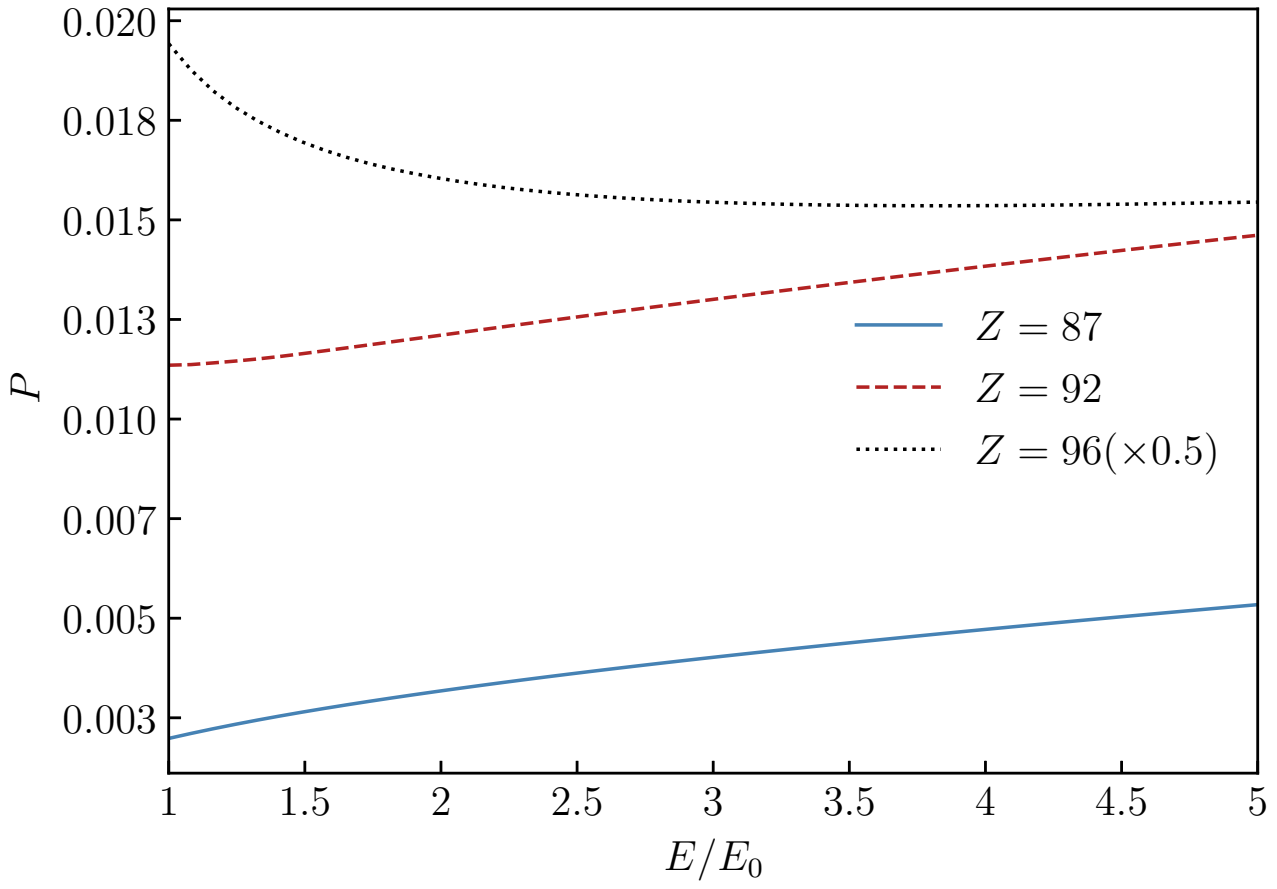
# How to observe the vacuum decay

*(I.A. Maltsev et al., PRL, 2019; R.V. Popov et al., PRD, 2020)*



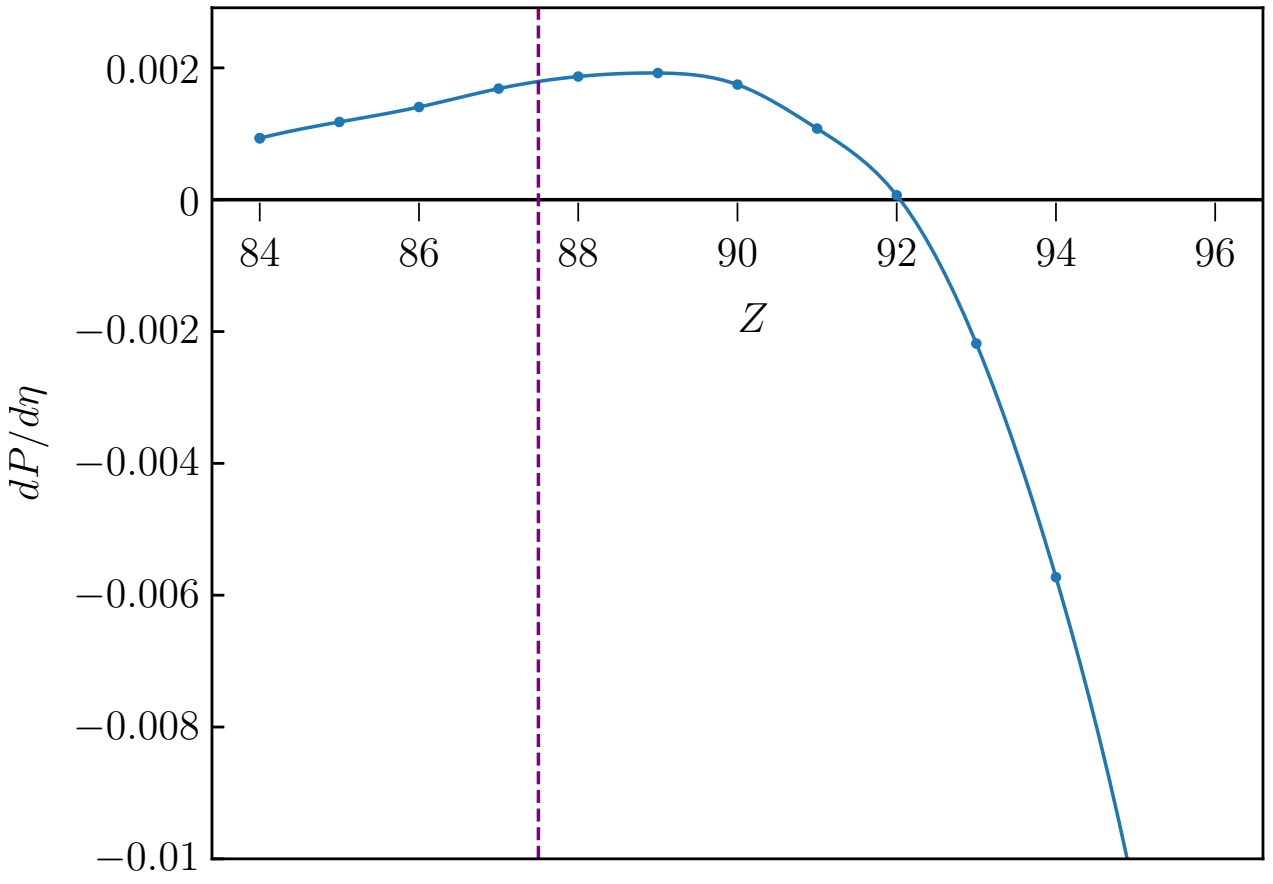

We consider only the trajectories for which the minimal internuclear distance is the same: $R_{\min} = 17.5$ fm. We introduce $\eta = E/E_0 \geq 1$.

## *How to observe the vacuum decay*




Total pair-production probability for symmetric ( $Z = Z_1 = Z_2$) collisions as a function of the collision energy at $R_{\min} = 17.5$ fm.

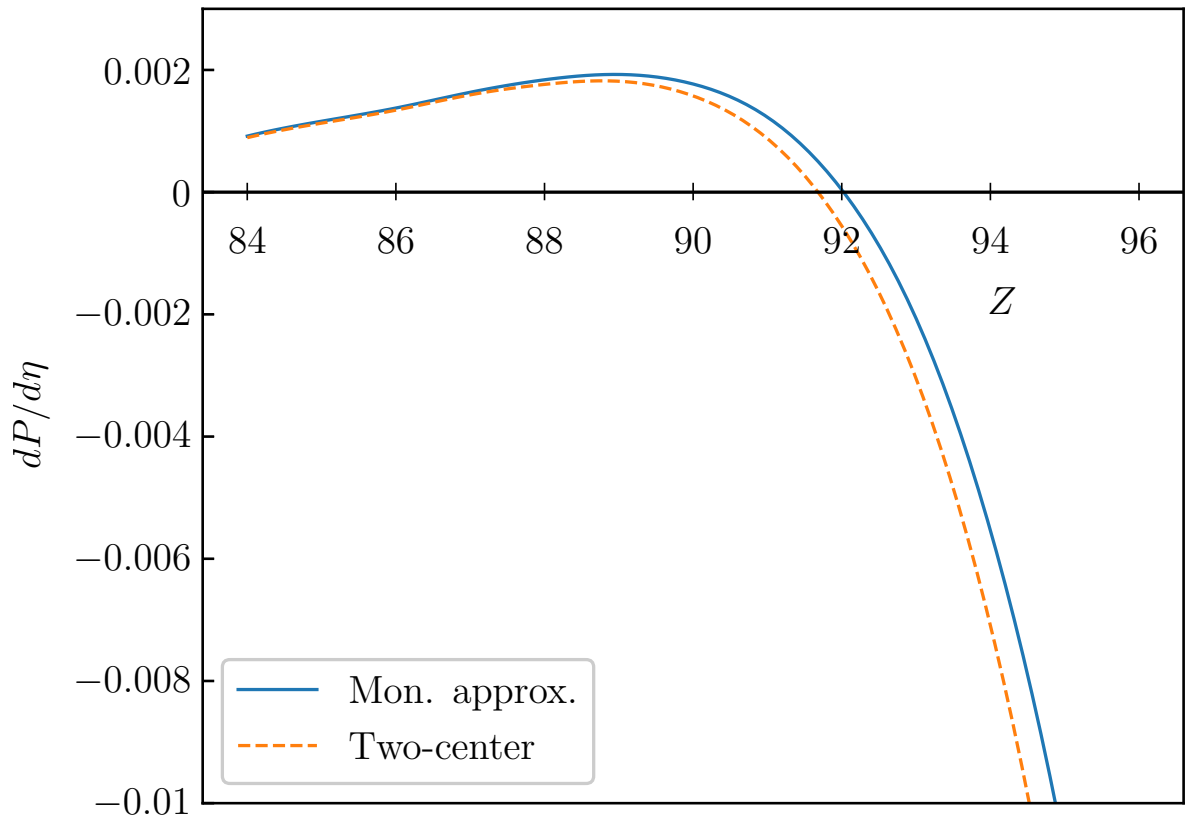
# How to observe the vacuum decay




The derivative of the pair-production probability with respect to the energy $dP/d\eta$, where $\eta = E/E_0$, at the point $\eta = 1$ as a function of the nuclear charge number $Z = Z_1 = Z_2$ at $R_{\min} = 17.5$ fm.

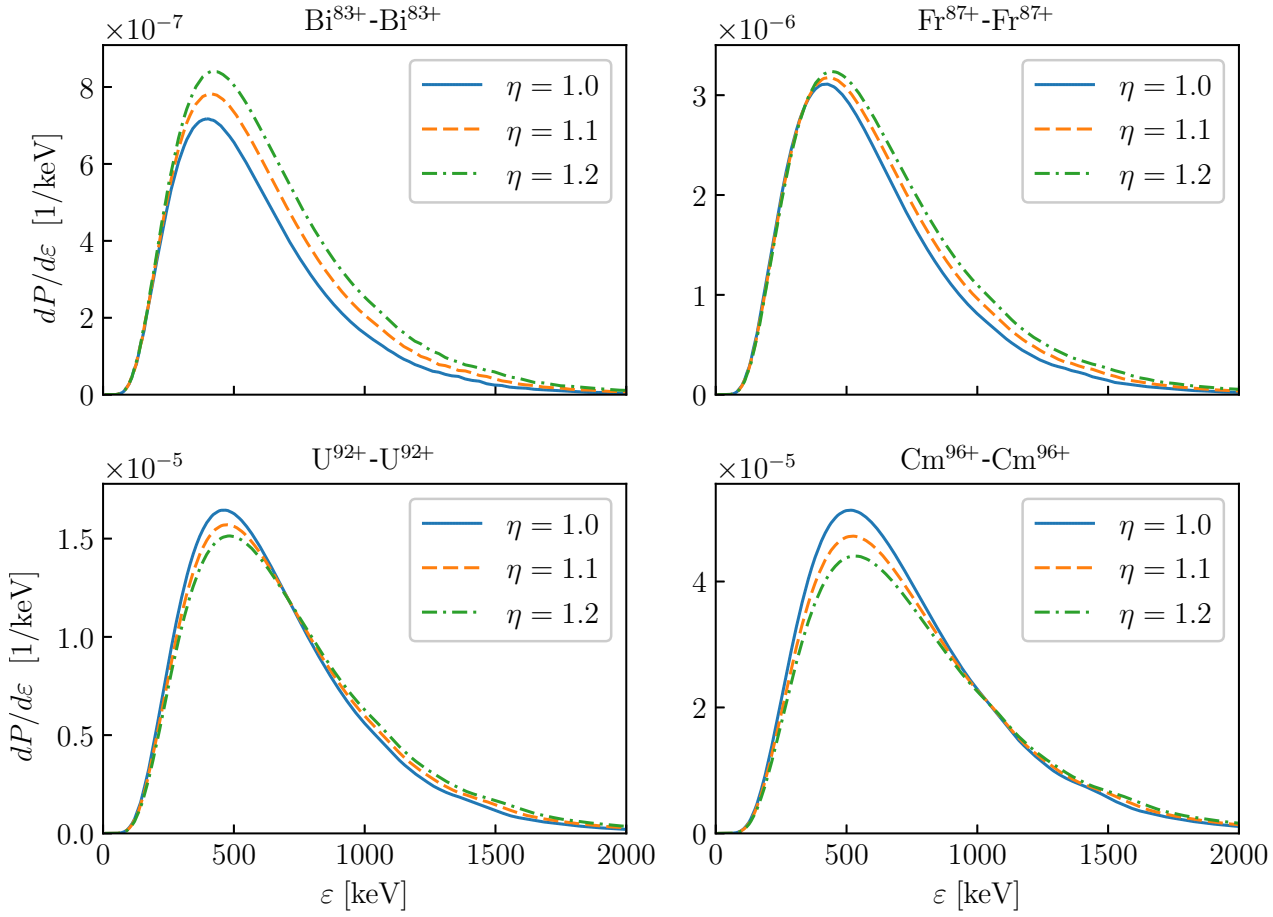
# How to observe the vacuum decay

Calculations beyond the monopole approximation
*(R.V. Popov, V.M. Shabaev, I.A. Maltsev et al., PRD, 2023)*



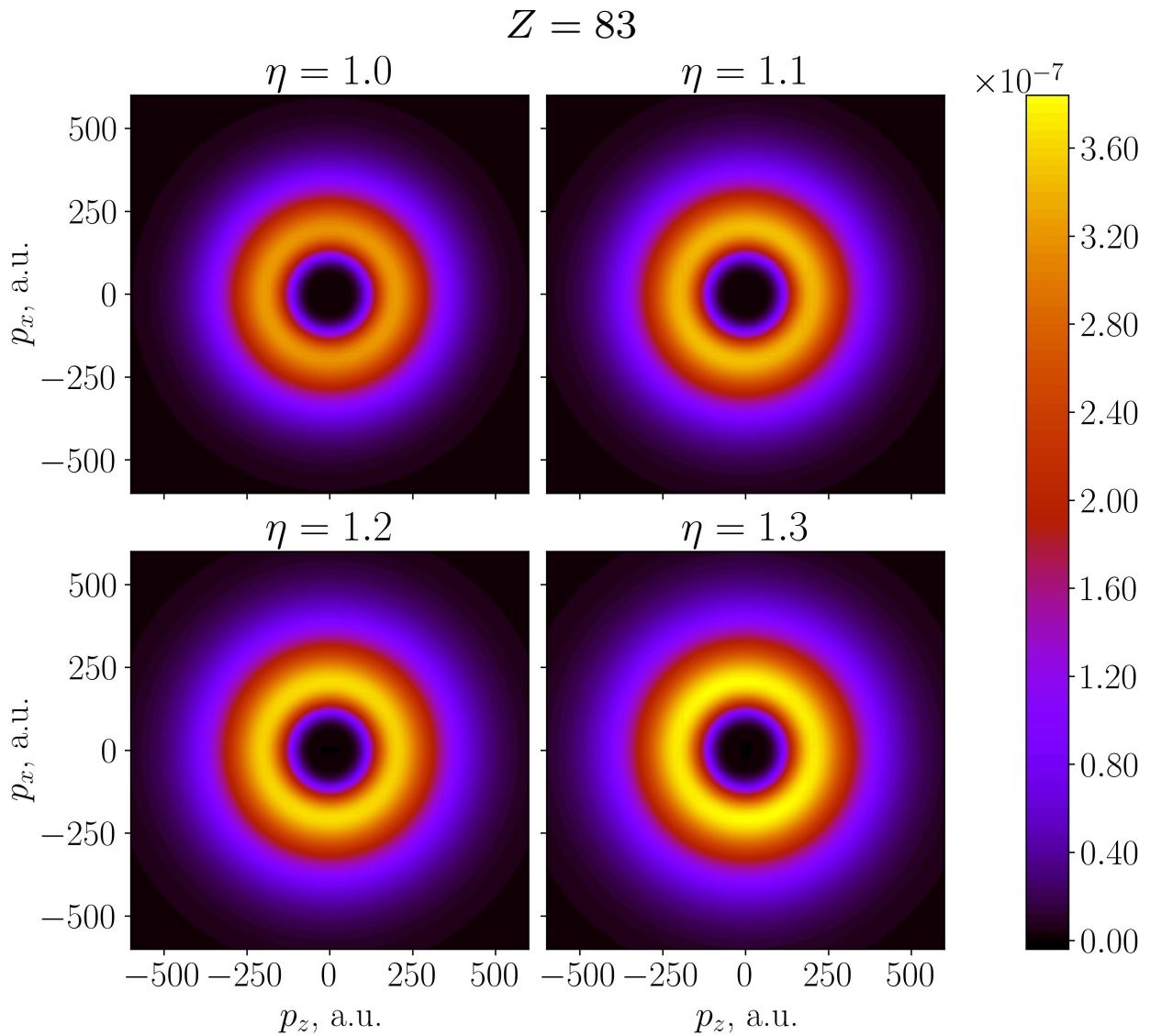

The derivative of the pair-production probability with respect to the energy $dP/d\eta$, where $\eta = E/E_0$, at the point $\eta = 1$ as a function of the nuclear charge number $Z = Z_1 = Z_2$ at $R_{\min} = 17.5$ fm.

# How to observe the vacuum decay



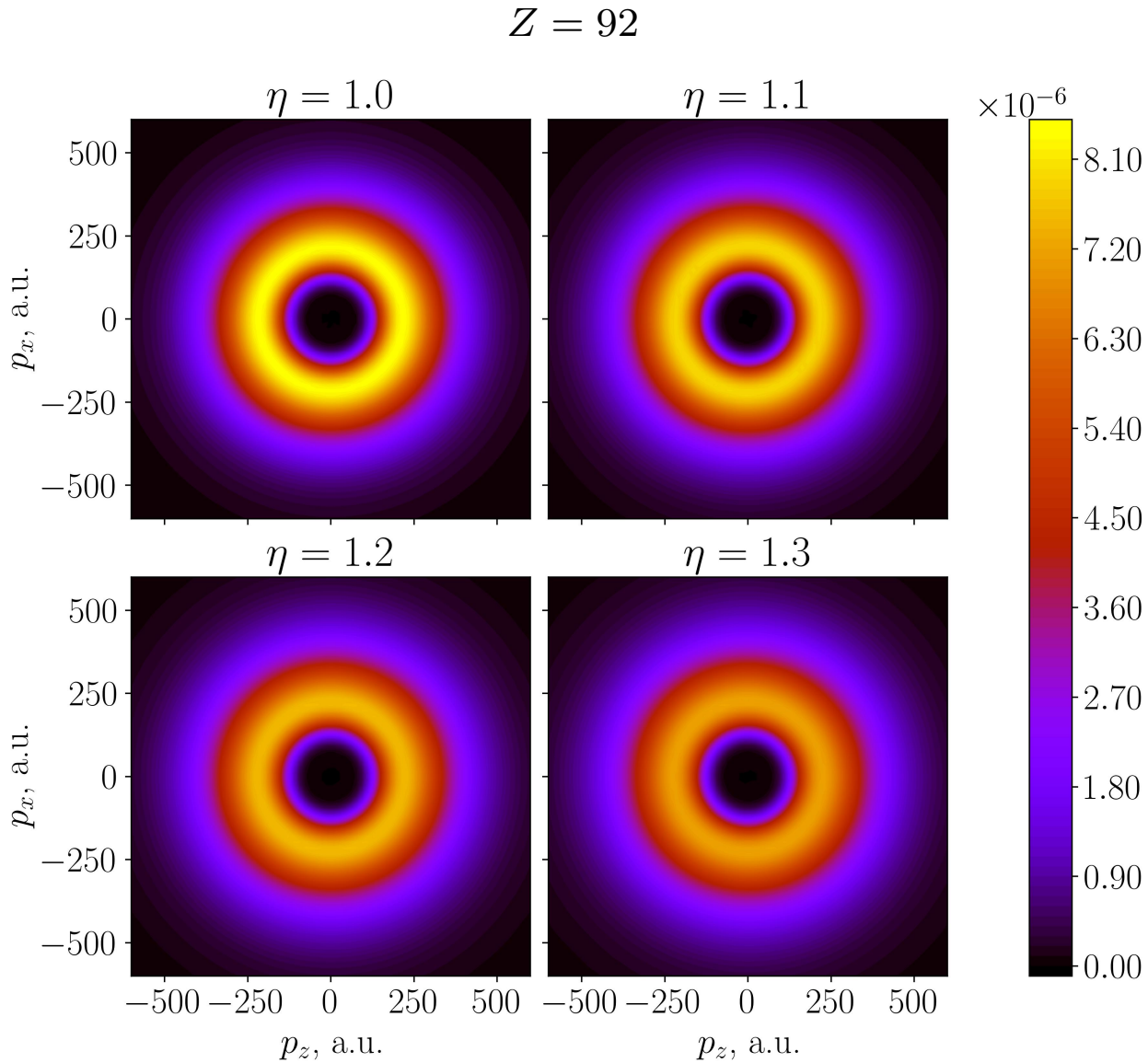

Positron spectra in symmetric ( $Z = Z_1 = Z_2$) collisions for different collision energy $\eta = E/E_0$ at $R_{\min} = 17.5$ fm.

# How to observe the vacuum decay




*N.K. Dulaev, D.A. Telnov, V.M. Shabaev et al., PRD, 2024.*

## How to observe the vacuum decay




*N.K. Dulaev, D.A. Telnov, V.M. Shabaev et al., PRD, 2024.*

## *How to observe the vacuum decay*

Background effects creating positrons *(W. Greiner et al., 1985)*

- Internal conversion of $\gamma$-rays from nuclear states
- External conversion of $\gamma$-rays in the target
- External conversion of $\gamma$-rays in the detector
- Conversion of $x$-rays from nuclear or electronic bremsstrahlung

All these background effects can either be kept under control or they can be neglected.

# Conclusion

**The results of the most recent calculations of SHEs are presented in:**

1) A. Ryzhkov, V. Pershina, M. Ilias, and V. Shabaev, Reactivity of Ts and At Oxides and Oxyhydrides with a Gold Surface from Periodic DFT Calculations, Phys. Chem. Chem. Phys. **26**, 9975 (2023).

2) I.I. Tupitsyn, I.M. Savelyev, A.V. Malyshev, Y.S. Kozhedub, D.A. Telnov, V.M. Shabaev, Orbital collapse of the 5g-electrons in the superheavy elements of the 8th period, Phys, Rev. A, **109**, 042807 (2024).

3) A.A. Kotov, Y.S. Kozhedub, D.A. Glazov, M. Ilias, V. Pershina, V.M. Shabaev, Relativistic calculations of spectroscopic properties of superheavy element compounds with H and OH radicals, in preparation.

**The most recent results on the vacuum decay are presented in:**

1) R.V. Popov, V.M. Shabaev, I.A. Maltsev, D.A. Telnov, N.K. Dulaev, and D.A. Tumakov, Spontaneous vacuum decay in low-energy collisions of heavy nuclei beyond the monopole approximation, Phys. Rev. D **107**, 116014 (2023).

2) D.A. Telnov, N.K. Dulaev, Y.S. Kozhedub, I.A. Maltsev, R.V. Popov, I.I. Tupitsyn, V.M. Shabaev, Positron supercritical resonances and spontaneous positron creation in slow collisions of heavy ions, Yad. Fiz., in press (2024).

3) N.K. Dulaev, D.A. Telnov, V.M. Shabaev, Y.S. Kozhedub, I.A. Maltsev, R.V. Popov, I.I. Tupitsyn, Angular and energy distributions of positrons created in subcritical and supercritical slow collisions of heavy nuclei, Phys. Rev. D **109**, 036008 (2024).

Thank You for Your Attention