

Reliable calculations of nuclear binding energies by the Gaussian process of machine learning*

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Reliable calculations of nuclear binding energies are crucial for advancing the research of nuclear physics. Machine learning provides an innovative approach to exploring complex physical problems. In this study, the nuclear binding energies are modeled directly using a machine-learning method called the Gaussian process. First, the binding energies for 2238 nuclei with $Z > 20$ and $N > 20$ are calculated using the Gaussian process in a physically motivated feature space, yielding an average deviation of 0.046 MeV and a standard deviation of 0.066 MeV. The results show the good learning ability of the Gaussian process in the studies of binding energies. Then, the predictive power of the Gaussian process is studied by calculating the binding energies for 108 nuclei newly included in AME2020. The theoretical results are in good agreement with the experimental data, reflecting the good predictive power of the Gaussian process. Moreover, the α -decay energies for 1169 nuclei with $50 \leq Z \leq 110$ are derived from the theoretical binding energies calculated using the Gaussian process. The average deviation and the standard deviation are, respectively, 0.047 MeV and 0.070 MeV. Noticeably, the calculated α -decay energies for the two new isotopes ^{204}Ac [M. H. Huang *et al.*, *Phys. Lett. B* **834**, 137484 (2022)] and ^{207}Th [H. B. Yang *et al.*, *Phys. Rev. C* **105**, L051302 (2022)] agree well with the latest experimental data. These results demonstrate that the Gaussian process is reliable for the calculations of nuclear binding energies. Finally, the α -decay properties of some unknown actinide nuclei are predicted using the Gaussian process. The predicted results can be useful guides for future research on binding energies and α -decay properties.

Keywords: nuclear binding energies, α decay, machine learning, Gaussian process

I. INTRODUCTION

Nuclear binding energies are important ground state properties that provide valuable information for probing nuclear structures [1–4] and serve as crucial inputs for some nuclear physics problems [5, 6]. For instance, binding energies play a key role in calculating the product cross sections for unknown nuclei using nuclear reaction models before synthesizing superheavy nuclei [7, 8]. They are also instrumental in identifying new nuclides in synthesis experiments of heavy and superheavy nuclei [9, 10] because α decay is one of the fundamental decay modes for most heavy and superheavy nuclei [11–13]. For α -emitters, there are two main α -decay observable properties, which are respectively α -decay energies and half-lives [14–18]. Thereinto, α -decay half-lives are strongly influenced by the α -decay energies, which can be calculated using the binding energies. Meanwhile, binding energies are also vital for calculating the properties of other radioactive decay modes, such as two-proton radioactivity [19] and heavy-cluster radioactivity [20]. Furthermore, the accuracy of binding energies has a significant impact on nuclear astrophysics studies, including r -process [21, 22], rp -process [23, 24], and the properties of neutron stars [25, 26]. Therefore, it is necessary to explore reliable theoretical models to calculate and predict the binding energies more accurately.

With the advancements in experimental nuclear physics facilities, binding energies of more than two thousand nuclei have been measured to date [27]. The accumulated experimental data provide a foundation for the development of theoretical models. In the past few years, numerous theoretical models and formulas have been proposed to calculate binding energies, including the Bethe-Weizsäcker formula [28, 29], the Thomas-Fermi (TF) model [30], the Hartree-Fock-Bogoliubov mean field model [31], and the finite-range drop model (FRDM) [32]. The theoretical binding energies calculated using these models and formulas are in good agreement with the experimental data. In Ref. [8], an improved binding-energy formula was proposed by incorporating additional physical terms into the standard Bethe-Weizsäcker formula, which consists of the shell effect and the neutron-proton correlations. The binding energies and α -decay energies can be well reproduced using this improved formula for heavy and superheavy nuclei with $Z \geq 90$ and $N \geq 140$. Although these current traditional models can provide theoretical guidance for studying binding energies, it is still worth exploring other models to provide more accurate calculations and predictions for future investigations of binding energies.

Machine learning has been widely used across many fields [33–38], as it can learn useful information from known systems and predict unknown properties within the same system using the obtained information. In the last decade, nuclear properties have been studied using various machine-learning methods based on available physical knowledge, including nuclear masses [39–41], nuclear charge radii [42], α -decay properties [43], and β -decay properties [44]. These nuclear properties can be well reproduced using machine learning. Recently, a new Bayesian machine learning mass model has been proposed [45], which can reproduce nuclear masses with the high accuracy required for the studies of r -process. As

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one of the popular machine-learning methods, the Gaussian process is a powerful nonparametric model, which is expected to model any distribution of the objectives [46]. Owing to its excellent flexibility in data modeling, the Gaussian process has been frequently applied in various studies [47, 48]. Notably, the Gaussian process can provide not only the theoretical values of the objectives but also the distribution of the calculated results, contributing to the visualization of the theoretical uncertainties [49]. Recently, the Gaussian process has been successfully exploited to predict the α -decay energies and half-lives of actinide nuclei [50]. Inspired by these previous works, it is of great interest to explore the reliability of the Gaussian process in the calculations of binding energies.

In this work, the Gaussian process has been extended to study the binding energies by directly modeling the experimental binding energies. The remainder of this paper is given as follows. In Sec. II, the theoretical framework, consisting of the Gaussian process with the modified kernel function and the physically motivated feature space, is provided. In Sec. III, the theoretical binding energies calculated using the Gaussian process are shown and discussed. Furthermore, the α -decay properties are reproduced and predicted based on the calculated binding energies. Finally, a comprehensive summary is presented in Sec. IV.

II. THEORETICAL FRAMEWORK

In the present work, the binding energy for a nucleus is considered as a realistic observation $B_p = b_p + \bar{\delta}$ with noise $\bar{\delta} \sim \mathcal{N}(0, \sigma_b^2)$. Here, $b_p = b(\mathbf{x}_p)$ is a latent function that denotes the noise-free binding energy for the p th nucleus \mathbf{x}_p [51]. B_p denotes the realistic binding energy, and $\bar{\delta}$ is an independently identically distributed Gaussian noise. Given a set of n nuclei with known binding energies into a training set $(\mathbf{x}_p, B_p)_{p=1}^n$, we aim to model the underlying physical relationship between each nucleus and its binding energy using the Gaussian process. Within the framework of the Gaussian process, the values of latent function $\mathbf{b} = (b_1, b_2, \dots, b_n)^T = (b(\mathbf{x}_1), b(\mathbf{x}_2), \dots, b(\mathbf{x}_n))^T$ are modeled by a joint Gaussian distribution, characterized by the values of a mean function $(m(\mathbf{x}_1), m(\mathbf{x}_2), \dots, m(\mathbf{x}_n))^T$ and the matrix of a covariance function $[k(\mathbf{x}_p, \mathbf{x}_q)]_{n \times n}$ [46]. Therefore, the Gaussian process can be generally denoted as $b(\mathbf{x}_p) \sim \mathcal{GP}(m(\mathbf{x}_p), k(\mathbf{x}_p, \mathbf{x}_q))$. The mean function $m(\mathbf{x}_p)$ is often set as zero because of the lack of prior knowledge. The so-called kernel function $k(\mathbf{x}_p, \mathbf{x}_q)$ can be written as a function of $|\mathbf{x}_p - \mathbf{x}_q|$, which is crucial for describing the similarities between pairs of nuclei. For the studies of binding energies, we choose a composite kernel function written as

$$k(\mathbf{x}_p, \mathbf{x}_q) = \eta_b^2 \left[\left(1 + \frac{\sqrt{3}r_b}{l_b} \right) \exp\left(-\frac{\sqrt{3}r_b}{l_b}\right) + \left(1 + \frac{r_b^2}{2\alpha_b d_b^2} \right)^{-\alpha_b} \right] \quad (1)$$

with $r_b = |\mathbf{x}_p - \mathbf{x}_q|$. The modified kernel function is a linear combination of two widely used kernel functions, which are the Matérn kernel function and the Rational Quadratic ker-

nel function, respectively. Here, η_b , l_b , α_b , and d_b are four hyperparameters of the Gaussian process. l_b , α_b , and d_b can capture the relevant range of the binding energies for pairs of nuclei, and η_b is able to describe the correlation intensity between them. For the realistic binding energy B_p , the covariance function becomes $k(\mathbf{x}_p, \mathbf{x}_q) \rightarrow k(\mathbf{x}_p, \mathbf{x}_q) + \sigma_b^2 \delta_{pq}$. δ_{pq} is a Kronecker delta where $\delta_{pq} = 1$ for $p = q$ and $\delta_{pq} = 0$ for $p \neq q$. When describing a number of nuclei $\mathbf{X} = (\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n)^T$, the binding energies $\mathbf{B} = (B_1, B_2, \dots, B_n)^T$ are expressed as $\mathbf{B} \sim \mathcal{GP}(\mathbf{0}, \mathbf{K}(\mathbf{X}, \mathbf{X}) + \sigma_b^2 \mathbf{I})$, where \mathbf{I} is a diagonal matrix.

The central interest of this work is to predict unknown binding energies based on the knowledge learned from the training set using the Gaussian process. When predicting unknown binding energies for nuclei \mathbf{X}_* with the training set $\mathcal{D} = (\mathbf{x}_p, B_p)_{p=1}^n$, the joint Gaussian distribution of the training outputs \mathbf{B} and the predicted outputs \mathbf{b}_* can be written as [46]

$$\begin{bmatrix} \mathbf{B} \\ \mathbf{b}_* \end{bmatrix} \sim \mathcal{N}\left(\mathbf{0}, \begin{bmatrix} \mathbf{K}(\mathbf{X}, \mathbf{X}) + \sigma_b^2 \mathbf{I} & \mathbf{K}(\mathbf{X}, \mathbf{X}_*) \\ \mathbf{K}(\mathbf{X}_*, \mathbf{X}) & \mathbf{K}(\mathbf{X}_*, \mathbf{X}_*) \end{bmatrix}\right). \quad (2)$$

For n_* predicted nuclei, $\mathbf{K}(\mathbf{X}, \mathbf{X})$, $\mathbf{K}(\mathbf{X}, \mathbf{X}_*)$, $\mathbf{K}(\mathbf{X}_*, \mathbf{X})$, and $\mathbf{K}(\mathbf{X}_*, \mathbf{X}_*)$, respectively, denote $n \times n$, $n \times n_*$, $n_* \times n$, and $n_* \times n_*$ matrix evaluated at all pairs of training and predicted points. By conditioning the joint Gaussian distribution, the crucial predicted expressions for the Gaussian process are $\mathbf{b}_* | \mathcal{D}, \mathbf{X}_* \sim \mathcal{N}(\mathbf{b}_*, \text{cov}(\mathbf{b}_*))$, where

$$\begin{aligned} \mathbf{b}_* &= \mathbf{K}(\mathbf{X}_*, \mathbf{X})[\mathbf{K}(\mathbf{X}, \mathbf{X}) + \sigma_b^2 \mathbf{I}]^{-1} \mathbf{B}, \\ \text{cov}(\mathbf{b}_*) &= \mathbf{K}(\mathbf{X}_*, \mathbf{X}_*) - \mathbf{K}(\mathbf{X}_*, \mathbf{X})[\mathbf{K}(\mathbf{X}, \mathbf{X}) + \sigma_b^2 \mathbf{I}]^{-1} \mathbf{K}(\mathbf{X}, \mathbf{X}_*). \end{aligned} \quad (3)$$

Here, the values of \mathbf{b}_* give the predicted binding energies for unknown nuclei. The variances of the predicted binding energies can be calculated by adding the noise variance σ_b^2 to the predictive variance given by $\text{cov}(\mathbf{b}_*)$.

As mentioned above, each nucleus is described by \mathbf{x}_p , which is a vector of physical features determining the description of the corresponding binding energy. In the present work, our goal is to obtain good descriptions of the binding energies using the Gaussian process with as simple physical information as possible. Hence, we construct a physical feature space with nine features, where $\mathbf{x}_p = (A_p, A_p^{2/3}, Z_p^2 A_p^{-1/3}, (A_p/2 - Z_p)^2/A_p, A_p^{-1/2}, \delta_p, |N_p - Z_p|/A_p, \pi_p, \nu_p)$. Here, A , Z , and N denote the mass, proton, and neutron numbers, respectively. The first six features are based on the Bethe-Weizsäcker formula [7, 28, 29, 52, 53]. A is introduced to model the proportional relationship between the binding energies and the nuclear volume, reflecting the saturation of nuclear force. $A^{2/3}$ is provided since the binding energies are expected to decrease on the nuclear surface. $Z^2 A^{-1/3}$ is used to describe the influence of the Coulomb interaction between protons. $(A/2 - Z)^2/A$ is the symmetry term that approximately estimates the balance between N and Z . $A^{-1/2}$ and $\delta = [(-1)^N + (-1)^Z]/2$ are used to describe the pairing energies with $\delta = 1, 0, -1$ for the even-even, odd- A , and odd-odd nuclei. $|N - Z|/A$ is from the Wigner term, which originates from the neutron-proton correlations [1, 8].

164 Additionally, π and v include the shell information, where
 165 π (v) is calculated using the numbers of protons (neutrons)
 166 away from the nearest proton (neutron) magic numbers [54].

167 The aforementioned theoretical framework implies that
 168 five hyperparameters need to be determined, which are η_b , l_b ,
 169 α_b , d_b , and σ_b , respectively. These can be determined by op-
 170 timizing the marginal likelihood using the training data [46].

171 III. NUMERICAL RESULTS AND DISCUSSIONS

172 In this section, we present and discuss the theoretical re-
 173 sults of the nuclear binding energies calculated using the
 174 Gaussian process. First, we calculate the binding ener-
 175 gies for nuclei with $Z > 20$ and $N > 20$ to evaluate
 176 the learning ability of the Gaussian process. The training
 177 set chosen in this work contains 2238 nuclei with known
 178 binding energies taken from AME2020 [55]. Each nucleus
 179 in the training set is presented as (\mathbf{x}_p, B_p) , where $\mathbf{x}_p =$
 180 $(A_p, A_p^{2/3}, Z_p^2 A_p^{-1/3}, (A_p/2 - Z_p)^2/A_p, A_p^{-1/2}, \delta_p, |N_p -$
 181 $Z_p|/A_p, \pi_p, v_p)$ and $B_p = B_p^{\text{Expt.}}$. After the training pro-
 182 cess, the hyperparameters are determined as $\eta_b = 1.814 \times$
 183 $10^4 \text{ MeV}^{1/2}$, $l_b = 1.821 \times 10^4$, $\alpha_b = 1937.218$, $d_b =$
 184 414.771 , and $\sigma_b = 0.093 \text{ MeV}^{1/2}$. The larger value of η_b in-
 185 dicates a stronger dependence between pairs of nuclei. Mean-
 186 while, the larger values of l_b , α_b , and d_b result in a relatively
 187 larger correlation range, which means that the change of bind-
 188 ing energies is comparatively smoother. Moreover, they also
 189 assist in avoiding the rapid growth of the error bars of the
 190 binding energies for nuclei away from the training data [46].

191 After the hyperparameters have been determined, the bind-
 192 ing energies can be calculated using the Gaussian process. To
 193 test the accuracy of the calculated results, we calculate the ab-
 194 solute value of the deviation between the experimental result
 195 and the theoretical one for each nucleus, defined by

$$196 \quad |\Delta_B| = |B_p^{\text{Expt.}} - B_p^{\text{Theo.}}|. \quad (4)$$

197 Here, $B_p^{\text{Expt.}}$ and $B_p^{\text{Theo.}}$ denote the experimental binding en-
 198 ergy and theoretical result calculated using the Gaussian pro-
 199 cess for the p th nucleus, respectively. The numerical results
 200 show that all absolute values of the deviations are smaller than
 201 0.423 MeV, indicating a small global deviation. We show the
 202 corresponding results in Fig. 1, in which the x- and y-axis in-
 203 dicate the neutron and proton numbers, respectively. The red
 204 squares depict the absolute values of the deviations, where
 205 darker colors are associated with larger deviations. The trans-
 206 verse and vertical dotted lines present $N = 28, 50, 82, 126$
 207 and $Z = 28, 50, 82$, respectively. It can be seen clearly from
 208 Fig. 1 that the colors of most squares are lighter, reflecting
 209 that the deviations for most nuclei are below 0.1 MeV. Addi-
 210 tionally, the binding energies for nuclei near the shell closure
 211 are also well reproduced using the Gaussian process. Next,
 212 we calculate the average deviation

$$213 \quad \langle \sigma_B \rangle = \frac{1}{\tilde{n}_B} \sum_{p=1}^{\tilde{n}_B} |B_p^{\text{Expt.}} - B_p^{\text{Theo.}}| \quad (5)$$

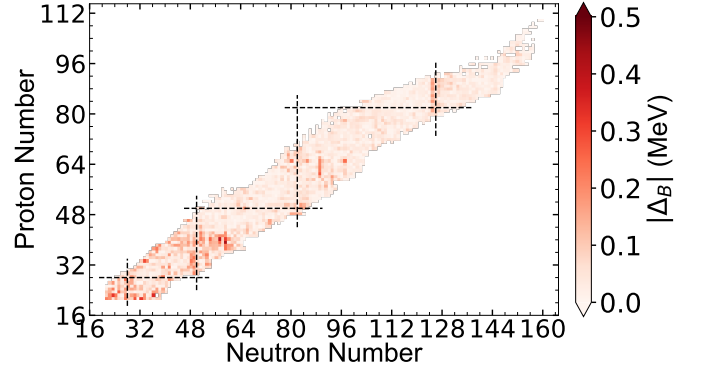


Fig. 1. The absolute values of deviations between experimen-
 tal binding energies and the theoretical results calculated using the
 Gaussian process across the nuclear chart. The darker colors indicate
 larger deviations of binding energies. Numerically, the largest
 absolute value of the deviations is $|\Delta_B| = 0.423 \text{ MeV}$.

214 and the standard deviation

$$215 \quad \sqrt{\sigma_B^2} = \sqrt{\frac{1}{\tilde{n}_B} \sum_{p=1}^{\tilde{n}_B} (B_p^{\text{Expt.}} - B_p^{\text{Theo.}})^2} \quad (6)$$

216 of the theoretical binding energies calculated using the Gaus-
 217 sian process for nuclei with $Z > 20$ and $N > 20$. Here,
 218 \tilde{n}_B denotes the number of nuclei included in the calcula-
 219 tions. The numerical values are $\langle \sigma_B \rangle = 0.046 \text{ MeV}$ and
 220 $\sqrt{\sigma_B^2} = 0.066 \text{ MeV}$, respectively. The small deviations
 221 show that the theoretical binding energies calculated using
 222 the Gaussian process with the modified kernel function in
 223 the physically motivated feature space are in good agreement
 224 with the experimental data. These results demonstrate the
 225 good learning ability of the Gaussian process in the studies
 226 of binding energies.

227 To further evaluate the learning ability and predictive
 228 power of the Gaussian process in the studies of binding en-
 229 ergies, we perform cross validation for the Gaussian process.
 230 In this work, we introduce the isotone-fold cross-validation
 231 that nuclei in each isotonic chain will be predicted using the
 232 Gaussian process based on the information provided by the
 233 remaining isotonic chains in the training set. The average de-
 234 viations and the standard deviations of the theoretical binding
 235 energies for nuclei in each isotonic chain are calculated, with
 236 results depicted in Fig. 2. For comparison, the average de-
 237 viations and the standard deviations of the binding energies cal-
 238 culated using the Bethe-Weizsäcker formula for each isotonic
 239 chain are also provided in Fig. 2. In Fig. 2(a) and Fig. 2(b),
 240 the red squares denote the average deviations and the standard
 241 deviations calculated using the Gaussian process for each iso-
 242 tonic chain, respectively. The blue circles present the average
 243 deviations and the standard deviations calculated using the
 244 Bethe-Weizsäcker formula for each isotonic chain separately.
 245 It is straightforward to see that the deviations given by the
 246 Gaussian process are quite small, which means that the cross-
 247 validation result is pretty good. In addition, we can find that
 248 the deviations are significantly reduced compared with those

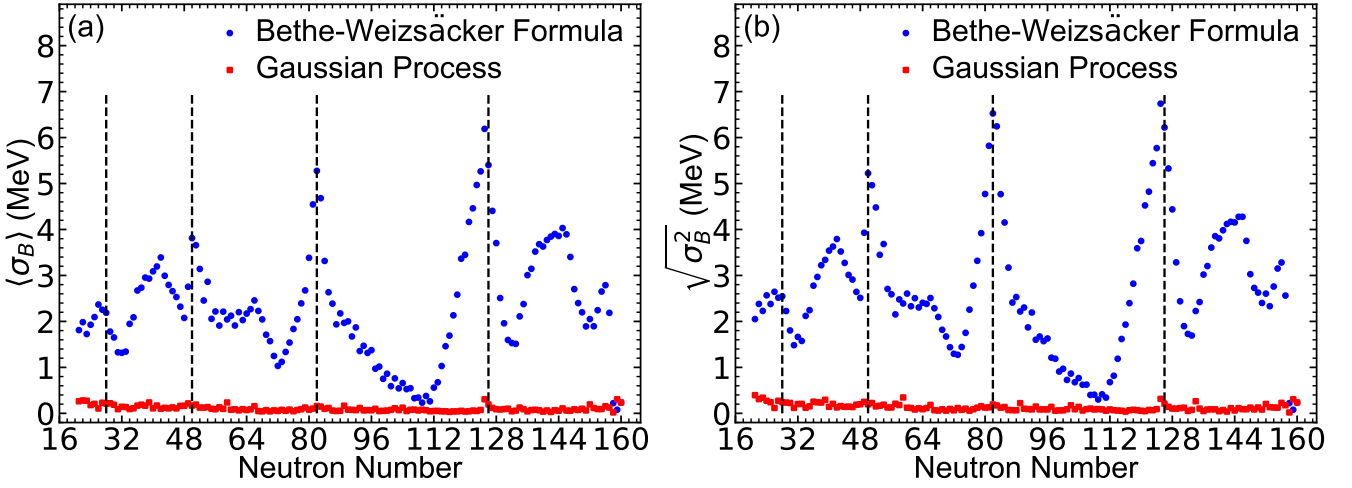


Fig. 2. The cross-validation results for nuclei in each isotopic chain calculated using the Gaussian process. In Fig. 2(a), the red squares and the blue circles depict the average deviations calculated using the Gaussian process and the Bethe-Weizsäcker formula, respectively. In Fig. 2(b), the red squares and the blue circles show the standard deviations calculated using the Gaussian process and the Bethe-Weizsäcker formula separately.

249 given by the Bethe-Weizsäcker formula. These results reflect
 250 the good learning ability and predictive power of the Gaussian
 251 process. Numerically, the total average deviation and standard
 252 deviation of the cross-validation for nuclei in the training
 253 set are $\langle \sigma_B \rangle = 0.100$ MeV and $\sqrt{\sigma_B^2} = 0.144$ MeV,
 254 respectively. The small deviations show that the predicted
 255 binding energies agree well with the experimental data, indicat-
 256 ing that the binding energies can be well learned using the
 257 Gaussian process. Thus, we can conclude that the learning
 258 ability and predictive power of the Gaussian process are
 259 reliable for studying the binding energies.

260 Then, we further test the predictive power of the Gaussian
 261 process by calculating the binding energies for nuclei that are
 262 present in AME2020 but not in AME2012 using the Gaussian
 263 process. To perform this calculation, the training set is chosen
 264 to include nuclei that are provided in both AME2012 and
 265 AME2020. Based on the training set, we predict the binding
 266 energies for 108 nuclei that are provided in AME2020 but
 267 not in AME2012 using the Gaussian process. The theoretical
 268 average deviation and standard deviation for these nuclei are
 269 $\langle \sigma_B \rangle = 0.216$ MeV and $\sqrt{\sigma_B^2} = 0.304$ MeV, respec-
 270 tively. These deviations are acceptable results in the calcula-
 271 tions of binding energies, verifying that the predicted power
 272 of the Gaussian process is commendable. Therefore, based on
 273 these theoretical results, it can be concluded that the Gaussian
 274 process is a reliable model for the studies of nuclear binding
 275 energies.

276 Next, we would like to calculate and discuss the theoret-
 277 ical results calculated using the Gaussian process with dif-
 278 ferent kernel functions and physical feature spaces. First,
 279 we calculate the binding energies using the Gaussian pro-
 280 cess with the Matérn kernel function and the Rational
 281 Quadratic kernel function, respectively. The correspond-
 282 ing deviations of the binding energies for 2238 nuclei are
 283 $(\langle \sigma_B \rangle, \sqrt{\sigma_B^2}) = (0.059, 0.076)$ MeV for the Matérn ker-

284 nel function and $(\langle \sigma_B \rangle, \sqrt{\sigma_B^2}) = (0.121, 0.166)$ MeV
 285 for the Rational Quadratic kernel function, respectively.
 286 The deviations for 108 new nuclei are $(\langle \sigma_B \rangle, \sqrt{\sigma_B^2}) =$
 287 $(0.278, 0.415)$ MeV for the Matérn kernel function and
 288 $(\langle \sigma_B \rangle, \sqrt{\sigma_B^2}) = (0.193, 0.249)$ MeV for the Rational
 289 Quadratic kernel function separately. Comparing with the devi-
 290 ations $(\langle \sigma_B \rangle, \sqrt{\sigma_B^2}) = (0.046, 0.066)$ MeV for 2238 nu-
 291 clei and $(\langle \sigma_B \rangle, \sqrt{\sigma_B^2}) = (0.216, 0.304)$ MeV for 108 new
 292 nuclei calculated using the composite kernel function, it can
 293 be found that the deviations calculated with the composite
 294 kernel function are as small as those calculated using the
 295 Matérn kernel function for 2238 nuclei and show better re-
 296 sults than those calculated using the Matérn kernel function
 297 for 108 new nuclei. The deviations calculated using the com-
 298 posite kernel function show results as good as those calcu-
 299 lated using the Rational Quadratic kernel function for 108
 300 new nuclei and are smaller than those calculated using the Ra-
 301 tional Quadratic kernel function for 2238 nuclei. Therefore,
 302 the good interpolation power of the Gaussian process with the
 303 Matérn kernel function and extrapolation ability of the
 304 Gaussian process with the Rational Quadratic kernel function
 305 are inherited by the composite kernel function in the calcula-
 306 tions of binding energies, which demonstrates that the mod-
 307 ified kernel function is a good choice for the present work.
 308 Furthermore, we hope that the choice of the composite kernel
 309 function can provide a new idea for modeling other physical
 310 problems using the Gaussian process.

311 We continue to compare the average deviations and stan-
 312 dard deviations for 108 new nuclei using the Gaussian pro-
 313 cess in different physical feature spaces. We first calcu-
 314 late the deviations for nuclei using the Gaussian pro-
 315 cess in the feature space consisting of six features taken
 316 from the Bethe-Weizsäcker formula, where the p th nu-
 317 cleus is described by $\mathbf{x}_p = (A_p, A_p^{2/3}, Z_p^2 A_p^{-1/3}, (A_p/2 -$

$Z_p)^2/A_p, A_p^{-1/2}, \delta_p)$. The theoretical deviations are
 $(\langle\sigma_B\rangle, \sqrt{\sigma_B^2}) = (0.437, 0.775)$ MeV. Then, we add the
neutron-proton correlation and the shell information in the
above feature space and compare the corresponding deviations.
When the neutron-proton correlation is added in the
feature space where $\mathbf{x}_p = (A_p, A_p^{2/3}, Z_p^2 A_p^{-1/3}, (A_p/2 -$
 $Z_p)^2/A_p, A_p^{-1/2}, \delta_p, |N_p - Z_p|/A_p)$, the deviations become
 $(\langle\sigma_B\rangle, \sqrt{\sigma_B^2}) = (0.398, 0.712)$ MeV. The reduction in the
deviations shows that the neutron-proton correlation is nec-
essary for calculating the binding energies. When the shell
information is included in the feature space, where $\mathbf{x}_p =$
 $(A_p, A_p^{2/3}, Z_p^2 A_p^{-1/3}, (A_p/2 - Z_p)^2/A_p, A_p^{-1/2}, \delta_p, \pi_p, \nu_p)$,
the deviations are $(\langle\sigma_B\rangle, \sqrt{\sigma_B^2}) = (0.236, 0.365)$ MeV. The
results reflect that the introduced features π and ν provide
useful shell information for nuclei in the calculations of bind-
ing energies. Furthermore, it can be observed that the above
deviations are larger than those calculated in the feature space
with nine features established in the present work, indicating
that our choice of feature space is reasonable. Notably, the
importance of the physically motivated feature space has also
been studied in the Bayesian neural network and the proba-
bilistic Mixture Density Network [39, 41]. The physical fea-
ture space established in the present work is first studied in
the Gaussian process on the research of binding energies.
It has been mentioned that the distribution of theoretical
results can be provided by the Gaussian process. Here, we
present the intervals of error bars for the theoretical results
calculated in this work. The lengths of error bars at 95%
confidence interval range from 0.213 MeV to 0.258 MeV in
the studies of 2238 nuclei, while they range from 0.234 MeV
to 4.022 MeV in the calculations of 108 new nuclei. These
results show that the hyperparameters determined by the
marginal likelihood are reasonable and that the theoretical
binding energies calculated using the Gaussian process are
reliable. Thus, we conclude that the Gaussian process with a
modified kernel function and the physically motivated feature
space is a reliable model for calculating binding energies.

Table 1: The theoretical α -decay energies calculated using the Gaus-
sian process for some actinide nuclei. The first column denotes the
actinide nuclei. The second and third columns list the experimen-
tal α -decay energies and the theoretical values calculated using the
Gaussian process separately. The last column presents the deviations
 $\Delta Q_\alpha = Q_\alpha^{\text{Expt.}} - Q_\alpha^{\text{Theo.}}$. The experimental data for the new nuclides
 ^{204}Ac and ^{207}Th are taken from Ref. [57] and Ref. [10], respectively.

| Nucl. | $Q_\alpha^{\text{Expt.}}$ (MeV) | $Q_\alpha^{\text{Theo.}}$ (MeV) | ΔQ_α (MeV) |
|------------------------|---------------------------------|---------------------------------|-------------------------|
| ^{204}Ac [57] | 8.107 | 8.107 | 0.000 |
| ^{205}Ac | 8.093 | 8.083 | 0.010 |
| ^{206}Ac | 7.958 | 7.943 | 0.015 |
| ^{207}Ac | 7.845 | 7.863 | -0.018 |
| ^{208}Ac | 7.729 | 7.736 | -0.007 |
| ^{209}Ac | 7.730 | 7.703 | 0.027 |
| ^{210}Ac | 7.586 | 7.608 | -0.022 |
| ^{211}Ac | 7.568 | 7.569 | -0.001 |

Table 1: (continued)

| Nucl. | $Q_\alpha^{\text{Expt.}}$ (MeV) | $Q_\alpha^{\text{Theo.}}$ (MeV) | ΔQ_α (MeV) |
|------------------------|---------------------------------|---------------------------------|-------------------------|
| ^{212}Ac | 7.540 | 7.490 | 0.050 |
| ^{213}Ac | 7.498 | 7.491 | 0.007 |
| ^{214}Ac | 7.352 | 7.531 | -0.179 |
| ^{215}Ac | 7.746 | 7.718 | 0.028 |
| ^{216}Ac | 9.241 | 9.012 | 0.229 |
| ^{217}Ac | 9.832 | 9.931 | -0.099 |
| ^{218}Ac | 9.384 | 9.437 | -0.053 |
| ^{219}Ac | 8.826 | 8.818 | 0.008 |
| ^{220}Ac | 8.348 | 8.324 | 0.024 |
| ^{221}Ac | 7.791 | 7.741 | 0.050 |
| ^{222}Ac | 7.137 | 7.226 | -0.089 |
| ^{223}Ac | 6.783 | 6.761 | 0.022 |
| ^{224}Ac | 6.327 | 6.318 | 0.009 |
| ^{225}Ac | 5.935 | 5.924 | 0.011 |
| ^{226}Ac | 5.506 | 5.483 | 0.023 |
| ^{227}Ac | 5.042 | 5.115 | -0.073 |
| ^{228}Ac | 4.721 | 4.697 | 0.024 |
| ^{229}Ac | 4.444 | 4.382 | 0.062 |
| ^{230}Ac | 3.893 | 3.934 | -0.041 |
| ^{231}Ac | 3.655 | 3.679 | -0.024 |
| ^{232}Ac | 3.345 | 3.345 | 0.000 |
| ^{233}Ac | 3.215 | 3.197 | 0.018 |
| ^{234}Ac | 2.930 | 2.942 | -0.012 |
| ^{235}Ac | 2.852 | 2.886 | -0.034 |
| ^{236}Ac | 2.723 | 2.668 | 0.055 |
| ^{207}Th [10] | 8.328 | 8.277 | 0.051 |
| ^{208}Th | 8.202 | 8.210 | -0.008 |
| ^{210}Th | 8.069 | 8.065 | 0.004 |
| ^{211}Th | 7.937 | 7.947 | -0.010 |
| ^{212}Th | 7.958 | 7.927 | 0.031 |
| ^{213}Th | 7.837 | 7.817 | 0.020 |
| ^{214}Th | 7.827 | 7.813 | 0.014 |
| ^{215}Th | 7.665 | 7.840 | -0.175 |
| ^{216}Th | 8.072 | 8.056 | 0.016 |
| ^{217}Th | 9.435 | 9.184 | 0.251 |
| ^{218}Th | 9.849 | 9.971 | -0.122 |
| ^{219}Th | 9.506 | 9.531 | -0.025 |
| ^{220}Th | 8.973 | 8.994 | -0.021 |
| ^{221}Th | 8.625 | 8.595 | 0.030 |
| ^{222}Th | 8.133 | 8.084 | 0.049 |
| ^{223}Th | 7.567 | 7.656 | -0.089 |
| ^{224}Th | 7.299 | 7.275 | 0.024 |
| ^{225}Th | 6.921 | 6.884 | 0.037 |

Table 1: (continued)

| Nucl. | $Q_{\alpha}^{\text{Expt.}}$ (MeV) | $Q_{\alpha}^{\text{Theo.}}$ (MeV) | ΔQ_{α} (MeV) |
|-------------------|-----------------------------------|-----------------------------------|---------------------------|
| ²²⁶ Th | 6.453 | 6.491 | -0.038 |
| ²²⁷ Th | 6.147 | 6.068 | 0.079 |
| ²²⁸ Th | 5.520 | 5.598 | -0.078 |
| ²²⁹ Th | 5.168 | 5.124 | 0.044 |
| ²³⁰ Th | 4.770 | 4.758 | 0.012 |
| ²³¹ Th | 4.213 | 4.289 | -0.076 |
| ²³² Th | 4.082 | 4.052 | 0.030 |
| ²³³ Th | 3.745 | 3.757 | -0.012 |
| ²³⁴ Th | 3.672 | 3.643 | 0.029 |
| ²³⁵ Th | 3.376 | 3.406 | -0.030 |
| ²³⁶ Th | 3.333 | 3.344 | -0.011 |
| ²³⁷ Th | 3.196 | 3.146 | 0.050 |
| ²¹¹ Pa | 8.481 | 8.467 | 0.014 |
| ²¹² Pa | 8.411 | 8.418 | -0.007 |
| ²¹³ Pa | 8.384 | 8.354 | 0.030 |
| ²¹⁴ Pa | 8.271 | 8.265 | 0.006 |
| ²¹⁵ Pa | 8.236 | 8.212 | 0.024 |
| ²¹⁶ Pa | 8.099 | 8.269 | -0.170 |
| ²¹⁷ Pa | 8.489 | 8.492 | -0.003 |
| ²¹⁸ Pa | 9.791 | 9.533 | 0.258 |
| ²¹⁹ Pa | 10.128 | 10.233 | -0.105 |
| ²²⁰ Pa | 9.704 | 9.762 | -0.058 |
| ²²¹ Pa | 9.248 | 9.225 | 0.023 |
| ²²² Pa | 8.789 | 8.784 | 0.005 |
| ²²³ Pa | 8.343 | 8.270 | 0.073 |
| ²²⁴ Pa | 7.694 | 7.788 | -0.094 |
| ²²⁵ Pa | 7.401 | 7.379 | 0.022 |
| ²²⁶ Pa | 6.987 | 6.965 | 0.022 |
| ²²⁷ Pa | 6.580 | 6.610 | -0.030 |
| ²²⁸ Pa | 6.265 | 6.226 | 0.039 |
| ²²⁹ Pa | 5.835 | 5.866 | -0.031 |
| ²³⁰ Pa | 5.439 | 5.432 | 0.007 |
| ²³¹ Pa | 5.150 | 5.102 | 0.048 |
| ²³² Pa | 4.627 | 4.658 | -0.031 |
| ²³³ Pa | 4.375 | 4.403 | -0.028 |
| ²³⁴ Pa | 4.076 | 4.110 | -0.034 |
| ²³⁵ Pa | 4.101 | 4.035 | 0.066 |
| ²³⁶ Pa | 3.755 | 3.810 | -0.055 |
| ²³⁷ Pa | 3.795 | 3.795 | 0.000 |
| ²³⁸ Pa | 3.628 | 3.573 | 0.055 |
| ²¹⁵ U | 8.588 | 8.569 | 0.019 |
| ²¹⁶ U | 8.531 | 8.570 | -0.039 |
| ²¹⁸ U | 8.775 | 8.840 | -0.065 |

Table 1: (continued)

| Nucl. | $Q_{\alpha}^{\text{Expt.}}$ (MeV) | $Q_{\alpha}^{\text{Theo.}}$ (MeV) | ΔQ_{α} (MeV) |
|-------------------|-----------------------------------|-----------------------------------|---------------------------|
| ²¹⁹ U | 9.950 | 9.780 | 0.170 |
| ²²¹ U | 9.889 | 9.965 | -0.076 |
| ²²² U | 9.481 | 9.459 | 0.022 |
| ²²³ U | 9.158 | 9.113 | 0.045 |
| ²²⁴ U | 8.628 | 8.580 | 0.048 |
| ²²⁵ U | 8.007 | 8.107 | -0.100 |
| ²²⁶ U | 7.701 | 7.662 | 0.039 |
| ²²⁷ U | 7.235 | 7.230 | 0.005 |
| ²²⁸ U | 6.800 | 6.828 | -0.028 |
| ²²⁹ U | 6.476 | 6.413 | 0.063 |
| ²³⁰ U | 5.992 | 6.030 | -0.038 |
| ²³¹ U | 5.576 | 5.608 | -0.032 |
| ²³² U | 5.414 | 5.345 | 0.069 |
| ²³³ U | 4.909 | 4.994 | -0.085 |
| ²³⁴ U | 4.858 | 4.860 | -0.002 |
| ²³⁵ U | 4.678 | 4.629 | 0.049 |
| ²³⁶ U | 4.573 | 4.551 | 0.022 |
| ²³⁷ U | 4.234 | 4.290 | -0.056 |
| ²³⁸ U | 4.270 | 4.273 | -0.003 |
| ²³⁹ U | 4.130 | 4.078 | 0.052 |
| ²⁴⁰ U | 4.035 | 4.067 | -0.032 |
| ²¹⁹ Np | 9.207 | 9.238 | -0.031 |
| ²²⁰ Np | 10.226 | 10.100 | 0.126 |
| ²²² Np | 10.200 | 10.222 | -0.022 |
| ²²³ Np | 9.650 | 9.664 | -0.014 |
| ²²⁴ Np | 9.329 | 9.323 | 0.006 |
| ²²⁵ Np | 8.818 | 8.765 | 0.053 |
| ²²⁶ Np | 8.328 | 8.363 | -0.035 |
| ²²⁷ Np | 7.816 | 7.847 | -0.031 |
| ²²⁹ Np | 7.020 | 7.061 | -0.041 |
| ²³⁰ Np | 6.778 | 6.757 | 0.021 |
| ²³¹ Np | 6.368 | 6.338 | 0.030 |
| ²³³ Np | 5.627 | 5.645 | -0.018 |
| ²³⁴ Np | 5.356 | 5.376 | -0.020 |
| ²³⁵ Np | 5.194 | 5.184 | 0.010 |
| ²³⁶ Np | 5.007 | 5.021 | -0.014 |
| ²³⁷ Np | 4.957 | 4.908 | 0.049 |
| ²³⁸ Np | 4.691 | 4.723 | -0.032 |
| ²³⁹ Np | 4.597 | 4.640 | -0.043 |
| ²⁴⁰ Np | 4.557 | 4.474 | 0.083 |
| ²⁴¹ Np | 4.363 | 4.363 | 0.000 |
| ²⁴² Np | 4.098 | 4.123 | -0.025 |
| ²²⁸ Pu | 7.940 | 7.910 | 0.030 |

Table 1: (continued)

| Nucl. | $Q_{\alpha}^{\text{Expt.}}$ (MeV) | $Q_{\alpha}^{\text{Theo.}}$ (MeV) | ΔQ_{α} (MeV) |
|-------------------|-----------------------------------|-----------------------------------|---------------------------|
| ²²⁹ Pu | 7.598 | 7.532 | 0.066 |
| ²³⁰ Pu | 7.178 | 7.207 | -0.029 |
| ²³¹ Pu | 6.839 | 6.890 | -0.051 |
| ²³² Pu | 6.716 | 6.689 | 0.027 |
| ²³³ Pu | 6.416 | 6.426 | -0.010 |
| ²³⁴ Pu | 6.310 | 6.261 | 0.049 |
| ²³⁵ Pu | 5.951 | 6.011 | -0.060 |
| ²³⁶ Pu | 5.867 | 5.883 | -0.016 |
| ²³⁷ Pu | 5.748 | 5.697 | 0.051 |
| ²³⁸ Pu | 5.593 | 5.555 | 0.038 |
| ²³⁹ Pu | 5.245 | 5.332 | -0.087 |
| ²⁴⁰ Pu | 5.256 | 5.248 | 0.008 |
| ²⁴¹ Pu | 5.140 | 5.094 | 0.046 |
| ²⁴² Pu | 4.984 | 4.982 | 0.002 |
| ²⁴³ Pu | 4.757 | 4.787 | -0.030 |
| ²⁴⁴ Pu | 4.666 | 4.661 | 0.005 |
| ²²⁹ Am | 8.137 | 8.123 | 0.014 |
| ²³⁵ Am | 6.576 | 6.622 | -0.046 |
| ²³⁶ Am | 6.256 | 6.378 | -0.122 |
| ²³⁸ Am | 6.042 | 6.038 | 0.004 |
| ²³⁹ Am | 5.922 | 5.909 | 0.013 |
| ²⁴⁰ Am | 5.707 | 5.731 | -0.024 |
| ²⁴¹ Am | 5.638 | 5.667 | -0.029 |
| ²⁴² Am | 5.589 | 5.519 | 0.070 |
| ²⁴³ Am | 5.439 | 5.413 | 0.026 |
| ²⁴⁴ Am | 5.138 | 5.207 | -0.069 |
| ²⁴⁵ Am | 5.160 | 5.152 | 0.008 |
| ²³³ Cm | 7.473 | 7.518 | -0.045 |
| ²³⁴ Cm | 7.365 | 7.382 | -0.017 |
| ²³⁶ Cm | 7.067 | 7.041 | 0.026 |
| ²³⁷ Cm | 6.770 | 6.815 | -0.045 |
| ²³⁸ Cm | 6.670 | 6.676 | -0.006 |
| ²³⁹ Cm | 6.540 | 6.498 | 0.042 |
| ²⁴⁰ Cm | 6.398 | 6.396 | 0.002 |
| ²⁴¹ Cm | 6.185 | 6.248 | -0.063 |
| ²⁴² Cm | 6.216 | 6.208 | 0.008 |
| ²⁴³ Cm | 6.169 | 6.083 | 0.086 |
| ²⁴⁴ Cm | 5.902 | 5.910 | -0.008 |
| ²⁴⁵ Cm | 5.624 | 5.657 | -0.033 |
| ²⁴⁶ Cm | 5.475 | 5.489 | -0.014 |
| ²⁴⁷ Cm | 5.354 | 5.311 | 0.043 |
| ²⁴⁸ Cm | 5.162 | 5.207 | -0.045 |
| ²⁴⁹ Cm | 5.148 | 5.154 | -0.006 |

Table 1: (continued)

| Nucl. | $Q_{\alpha}^{\text{Expt.}}$ (MeV) | $Q_{\alpha}^{\text{Theo.}}$ (MeV) | ΔQ_{α} (MeV) |
|-------------------|-----------------------------------|-----------------------------------|---------------------------|
| ²⁵⁰ Cm | 5.170 | 5.155 | 0.015 |
| ²³⁴ Bk | 8.099 | 7.882 | 0.217 |
| ²⁴³ Bk | 6.874 | 6.909 | -0.035 |
| ²⁴⁴ Bk | 6.779 | 6.724 | 0.055 |
| ²⁴⁵ Bk | 6.455 | 6.419 | 0.036 |
| ²⁴⁶ Bk | 6.074 | 6.149 | -0.075 |
| ²⁴⁷ Bk | 5.890 | 5.896 | -0.006 |
| ²⁴⁸ Bk | 5.827 | 5.765 | 0.062 |
| ²⁴⁹ Bk | 5.521 | 5.610 | -0.089 |
| ²³⁷ Cf | 8.220 | 8.249 | -0.029 |
| ²³⁹ Cf | 7.763 | 7.886 | -0.123 |
| ²⁴⁰ Cf | 7.711 | 7.745 | -0.034 |
| ²⁴² Cf | 7.517 | 7.541 | -0.024 |
| ²⁴⁴ Cf | 7.329 | 7.337 | -0.008 |
| ²⁴⁵ Cf | 7.258 | 7.169 | 0.089 |
| ²⁴⁶ Cf | 6.862 | 6.862 | 0.000 |
| ²⁴⁷ Cf | 6.503 | 6.585 | -0.082 |
| ²⁴⁸ Cf | 6.361 | 6.358 | 0.003 |
| ²⁴⁹ Cf | 6.293 | 6.263 | 0.030 |
| ²⁵⁰ Cf | 6.129 | 6.174 | -0.045 |
| ²⁵¹ Cf | 6.177 | 6.175 | 0.002 |
| ²⁵² Cf | 6.217 | 6.166 | 0.051 |
| ²⁵³ Cf | 6.126 | 6.166 | -0.040 |
| ²⁵⁴ Cf | 5.927 | 5.915 | 0.012 |
| ²⁴¹ Es | 8.259 | 8.336 | -0.077 |
| ²⁴² Es | 8.160 | 8.062 | 0.098 |
| ²⁴³ Es | 8.072 | 7.905 | 0.167 |
| ²⁴⁵ Es | 7.909 | 7.610 | 0.299 |
| ²⁴⁷ Es | 7.464 | 7.378 | 0.086 |
| ²⁵¹ Es | 6.597 | 6.709 | -0.112 |
| ²⁵² Es | 6.739 | 6.702 | 0.037 |
| ²⁵³ Es | 6.739 | 6.683 | 0.056 |
| ²⁵⁴ Es | 6.617 | 6.676 | -0.059 |
| ²⁵⁵ Es | 6.436 | 6.415 | 0.021 |
| ²⁴³ Fm | 8.689 | 9.127 | -0.438 |
| ²⁴⁶ Fm | 8.379 | 8.391 | -0.012 |
| ²⁴⁷ Fm | 8.258 | 8.105 | 0.153 |
| ²⁴⁸ Fm | 7.995 | 7.980 | 0.015 |
| ²⁴⁹ Fm | 7.709 | 7.713 | -0.004 |
| ²⁵⁰ Fm | 7.557 | 7.563 | -0.006 |
| ²⁵¹ Fm | 7.424 | 7.359 | 0.065 |
| ²⁵² Fm | 7.154 | 7.255 | -0.101 |
| ²⁵³ Fm | 7.198 | 7.192 | 0.006 |

Table 1: (continued)

| Nucl. | $Q_{\alpha}^{\text{Expt.}}$ (MeV) | $Q_{\alpha}^{\text{Theo.}}$ (MeV) | ΔQ_{α} (MeV) |
|-------------------|-----------------------------------|-----------------------------------|---------------------------|
| ²⁵⁴ Fm | 7.307 | 7.256 | 0.051 |
| ²⁵⁵ Fm | 7.241 | 7.259 | -0.018 |
| ²⁵⁶ Fm | 7.025 | 7.032 | -0.007 |
| ²⁵⁷ Fm | 6.864 | 6.882 | -0.018 |
| ²⁴⁶ Md | 8.889 | 9.193 | -0.304 |
| ²⁴⁷ Md | 8.764 | 8.983 | -0.219 |
| ²⁴⁸ Md | 8.497 | 8.647 | -0.150 |
| ²⁵⁰ Md | 8.155 | 8.135 | 0.020 |
| ²⁵¹ Md | 7.963 | 7.982 | -0.019 |
| ²⁵³ Md | 7.573 | 7.814 | -0.241 |
| ²⁵⁵ Md | 7.906 | 7.834 | 0.072 |
| ²⁵⁷ Md | 7.557 | 7.505 | 0.052 |
| ²⁵⁸ Md | 7.271 | 7.263 | 0.008 |
| ²⁵¹ No | 8.752 | 8.833 | -0.081 |
| ²⁵² No | 8.549 | 8.555 | -0.006 |
| ²⁵³ No | 8.415 | 8.406 | 0.009 |
| ²⁵⁴ No | 8.226 | 8.327 | -0.101 |
| ²⁵⁵ No | 8.428 | 8.413 | 0.015 |
| ²⁵⁶ No | 8.582 | 8.480 | 0.102 |
| ²⁵⁷ No | 8.477 | 8.496 | -0.019 |
| ²⁵⁹ No | 7.854 | 7.859 | -0.005 |

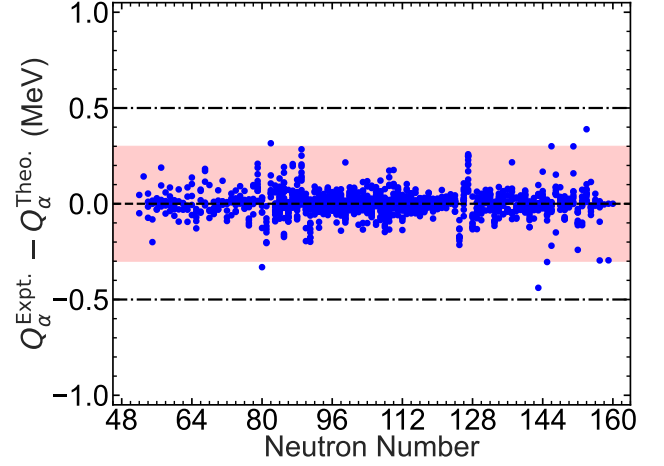


Fig. 3. The deviations between the experimental α -decay energies and the theoretical results for 1169 nuclei with $50 \leq Z \leq 110$. The blue circles depict the deviations for these nuclei. The dashed line denotes $|Q_{\alpha}^{\text{Expt.}} - Q_{\alpha}^{\text{Theo.}}| = 0$ MeV. The red shadow and the dash dotted lines present $|Q_{\alpha}^{\text{Expt.}} - Q_{\alpha}^{\text{Theo.}}| \leq 0.3$ MeV and $|Q_{\alpha}^{\text{Expt.}} - Q_{\alpha}^{\text{Theo.}}| = 0.5$ MeV, respectively.

382 given by

$$383 \quad \langle \sigma_{\alpha} \rangle = \frac{1}{\tilde{n}_{\alpha}} \sum_{p=1}^{\tilde{n}_{\alpha}} |Q_{\alpha}^{\text{Expt.},p} - Q_{\alpha}^{\text{Theo.},p}| = 0.047 \text{ MeV} \quad (7)$$

384 and

$$385 \quad \sqrt{\sigma_{\alpha}^2} = \sqrt{\frac{1}{\tilde{n}_{\alpha}} \sum_{p=1}^{\tilde{n}_{\alpha}} (Q_{\alpha}^{\text{Expt.},p} - Q_{\alpha}^{\text{Theo.},p})^2} = 0.070 \text{ MeV}. \quad (8)$$

386 Owing to the complexity of the quantum many-body theory, it is difficult to calculate the α -decay energies with deviations less than 0.1 MeV. These small deviations show that the α -decay energies agree well with the experimental results.

389 Recently, some actinide nuclei, including ²⁰⁴Ac [57] and ²⁰⁷Th [10], were synthesized experimentally. Theoretical α -decay properties provide useful references for these experiments. Here, we present the theoretical α -decay energies calculated using the Gaussian process for the actinide nuclei in Table 1. In Table 1, the first column lists the actinide nuclei. The second column denotes the experimental data and the third column presents the theoretical results. The fourth column gives the deviations $\Delta Q_{\alpha} = Q_{\alpha}^{\text{Expt.}} - Q_{\alpha}^{\text{Theo.}}$ between the experimental results and the theoretical ones. The experimental α -decay energies for two new nuclides ²⁰⁴Ac and ²⁰⁷Th are taken from Ref. [57] and Ref. [10] separately. It can be clearly seen that the theoretical results obtained using the Gaussian process are in good agreement with the experimental data for the actinide nuclei. For the new nuclide ²⁰⁴Ac, the theoretical α -decay energy calculated using the Gaussian process is nearly equivalent to the experimental result, with a small deviation of $\Delta Q_{\alpha} = Q_{\alpha}^{\text{Expt.}} - Q_{\alpha}^{\text{Theo.}} = 0.0004$ MeV. For another new nuclide, ²⁰⁷Th, the deviation is

355 Due to the successful calculations of the binding energies, it is expected that the α -decay energies, which are the differences among the binding energies of the parent nuclei, the daughter nuclei, and the α -particles, can be reproduced with good accuracy. Thus, we calculate the α -decay energies for 1169 nuclei with $50 \leq Z \leq 110$ and compare the calculated results with the experimental data taken from AME2020 [27]. The deviations between the experimental α -decay energies and the theoretical results for these nuclei are depicted in Fig. 3. In Fig. 3, the blue circles denote the deviations and the red shadow shows the deviations $|Q_{\alpha}^{\text{Expt.}} - Q_{\alpha}^{\text{Theo.}}| \leq 0.3$ MeV. The dashed line represents $|Q_{\alpha}^{\text{Expt.}} - Q_{\alpha}^{\text{Theo.}}| = 0$ MeV and the two dash dotted lines present $|Q_{\alpha}^{\text{Expt.}} - Q_{\alpha}^{\text{Theo.}}| = 0.5$ MeV, respectively. The deviations for the α -decay energies of the 1169 nuclei are all clearly below 0.5 MeV and the deviations for most of these nuclei are less than 0.3 MeV. These results show good agreement between the theoretical α -decay energies derived from the binding energies which are calculated using the Gaussian process and the experimental data. Furthermore, it has been found in previous studies that α -decay energies are strongly affected by the shell effect, which leads to larger deviations for nuclei near the closed shell [56]. In Fig. 3, the deviations for nuclei near the shell closure are also less than 0.3 MeV. It can reflect that π and ν features can successfully model the shell effect with the Gaussian process. We also calculate the average deviation and standard deviation for these nuclei,

409 $\Delta Q_\alpha = Q_\alpha^{\text{Expt.}} - Q_\alpha^{\text{Theo.}} = 0.051$ MeV, indicating that the
 410 calculated result is in good agreement with the experimental
 411 one. These results demonstrate that the α -decay energies for
 412 the actinide nuclei can be well reproduced by deriving from
 413 the theoretical binding energies calculated using the Gaussian
 414 process. Overall, the above results show the reliability of the
 415 Gaussian process in the calculations of nuclear binding ener-
 416 gies and α -decay properties.

Table 2: The predicted α -decay energies and half-lives for some un-
 known actinide nuclei. The first column denotes the α -decay emitters.
 The second and third columns are the predicted α -decay energies cal-
 culated using the Gaussian process and the FRDM separately. The
 fourth and fifth columns represent the predicted α -decay half-lives cal-
 culated using the NGNL with the predicted α -decay energies given by
 the Gaussian process and the FRDM, respectively. The units of the
 α -decay half-lives are seconds.

| Nucl. | Q_α^{GP} (MeV) | Q_α^{FRDM} (MeV) | $\log_{10}(T_{1/2}^{\text{GP}})$ | $\log_{10}(T_{1/2}^{\text{FRDM}})$ |
|-------------------|------------------------------|--------------------------------|----------------------------------|------------------------------------|
| ²⁰⁰ Ac | 9.260 | 8.905 | -4.982 | -4.089 |
| ²⁰¹ Ac | 9.016 | 8.895 | -4.373 | -4.062 |
| ²⁰² Ac | 8.639 | 8.685 | -3.383 | -3.507 |
| ²⁰³ Ac | 8.432 | 8.575 | -2.811 | -3.208 |
| ²⁰³ Th | 8.948 | 8.825 | -3.865 | -3.542 |
| ²⁰⁴ Th | 8.827 | 8.765 | -3.547 | -3.381 |
| ²⁰⁵ Th | 8.595 | 8.575 | -2.917 | -2.862 |
| ²⁰⁶ Th | 8.469 | 8.515 | -2.565 | -2.694 |
| ²⁰⁷ Pa | 8.495 | 8.765 | -2.289 | -3.040 |
| ²⁰⁸ Pa | 8.478 | 8.565 | -2.240 | -2.487 |
| ²⁰⁹ Pa | 8.461 | 8.305 | -2.191 | -1.738 |
| ²¹⁰ Pa | 8.456 | 8.265 | -2.176 | -1.619 |
| ²¹⁰ U | 8.456 | 8.605 | -1.825 | -2.252 |
| ²¹¹ U | 8.512 | 8.485 | -1.986 | -1.909 |
| ²¹² U | 8.490 | 8.365 | -1.922 | -1.558 |
| ²¹³ U | 8.542 | 8.385 | -2.071 | -1.617 |
| ²¹⁵ Np | 8.444 | 8.815 | -1.435 | -2.490 |
| ²¹⁶ Np | 8.544 | 8.625 | -1.726 | -1.958 |
| ²¹⁷ Np | 8.684 | 8.725 | -2.124 | -2.239 |
| ²¹⁸ Np | 8.956 | 8.945 | -2.872 | -2.842 |
| ²²⁴ Pu | 9.914 | 9.565 | -5.944 | -5.107 |
| ²²⁵ Pu | 9.306 | 9.285 | -4.455 | -4.401 |
| ²²⁶ Pu | 8.774 | 9.035 | -3.028 | -3.744 |
| ²²⁷ Pu | 8.246 | 8.695 | -1.476 | -2.804 |
| ²²⁵ Am | 9.977 | 9.895 | -5.779 | -5.587 |
| ²²⁶ Am | 9.348 | 9.605 | -4.235 | -4.884 |
| ²²⁷ Am | 8.936 | 9.345 | -3.136 | -4.227 |
| ²²⁸ Am | 8.423 | 9.075 | -1.657 | -3.515 |
| ²²⁹ Cm | 8.727 | 9.395 | -2.202 | -4.027 |
| ²³⁰ Cm | 8.419 | 8.725 | -1.288 | -2.196 |
| ²³¹ Cm | 8.068 | 8.385 | -0.182 | -1.183 |

Table 2: (continued)

| Nucl. | Q_α^{GP} (MeV) | Q_α^{FRDM} (MeV) | $\log_{10}(T_{1/2}^{\text{GP}})$ | $\log_{10}(T_{1/2}^{\text{FRDM}})$ |
|-------------------|------------------------------|--------------------------------|----------------------------------|------------------------------------|
| ²³² Cm | 7.788 | 7.885 | 0.753 | 0.424 |
| ²²⁹ Bk | 9.233 | 9.555 | -3.270 | -4.112 |
| ²³⁰ Bk | 8.864 | 9.165 | -2.249 | -3.086 |
| ²³¹ Bk | 8.549 | 8.805 | -1.326 | -2.080 |
| ²³² Bk | 8.270 | 8.465 | -0.464 | -1.070 |
| ²³³ Cf | 9.392 | 8.585 | -3.360 | -1.080 |
| ²³⁴ Cf | 9.092 | 8.665 | -2.548 | -1.319 |
| ²³⁵ Cf | 8.726 | 8.535 | -1.500 | -0.927 |
| ²³⁶ Cf | 8.509 | 8.335 | -0.847 | -0.305 |
| ²³⁷ Es | 9.679 | 8.645 | -3.778 | -0.906 |
| ²³⁸ Es | 9.215 | 8.485 | -2.548 | -0.415 |
| ²³⁹ Es | 8.935 | 8.155 | -1.760 | 0.643 |
| ²⁴⁰ Es | 8.558 | 7.975 | -0.639 | 1.248 |
| ²³⁹ Fm | 10.540 | 8.845 | -5.536 | -1.152 |
| ²⁴⁰ Fm | 10.260 | 8.605 | -4.887 | -0.428 |
| ²⁴¹ Fm | 9.791 | 8.405 | -3.739 | 0.199 |
| ²⁴² Fm | 9.548 | 8.285 | -3.110 | 0.586 |
| ²⁴² Md | 10.392 | 9.045 | -4.889 | -1.389 |
| ²⁴³ Md | 10.139 | 9.005 | -4.284 | -1.273 |
| ²⁴⁴ Md | 9.767 | 8.935 | -3.354 | -1.068 |
| ²⁴⁵ Md | 9.541 | 8.925 | -2.762 | -1.038 |
| ²⁴⁵ No | 10.326 | 9.505 | -4.423 | -2.336 |
| ²⁴⁶ No | 10.104 | 9.465 | -3.883 | -2.227 |
| ²⁴⁷ No | 9.878 | 9.335 | -3.316 | -1.869 |
| ²⁴⁸ No | 9.629 | 9.205 | -2.667 | -1.504 |

417 Finally, we predict the α -decay energies for some unknown
 418 actinide nuclei using the Gaussian process. With the pre-
 419 dicted α -decay energies, we also calculate the α -decay half-
 420 lives using the new Geiger-Nuttall law (NGNL) [58]. The
 421 corresponding results are given in Table 2. In Table 2, the first
 422 column lists the α -emitters. The second and third columns
 423 present the α -decay energies calculated using the Gaussian
 424 process and the FRDM, respectively. The fourth and fifth
 425 columns give the predictive α -decay half-lives calculated us-
 426 ing the NGNL with the α -decay energies predicted by the
 427 Gaussian process and the FRDM, respectively. It can be
 428 found that most predicted α -decay energies agree well with
 429 those calculated using the FRDM. Nevertheless, the predicted
 430 α -decay energies for Einsteinium, Fermium, Mendelevium,
 431 and Nobelium are relatively larger than those given by the
 432 FRDM, which results in different α -decay half-lives. We
 433 hope that future experimental α -decay properties for Ein-
 434 steinium, Fermium, Mendelevium, and Nobelium can pro-
 435 vide useful information for improving the Gaussian process.
 436 The α -decay properties predicted by the Gaussian process can
 437 complement existing theoretical models and provide valuable
 438 guidance for future studies of α decay. In addition, some ac-

tinide isotopes are being synthesized at the Heavy Ion Research Facility in Lanzhou (HIRFL), China. Therefore, it is expected that the predicted α -decay properties can be used as theoretical references for identifying new nuclides in the future.

IV. SUMMARY

In this work, the Gaussian process with a composite kernel function is applied to study the binding energies. First, we calculate the binding energies for 2238 nuclei with $Z > 20$ and $N > 20$ within the framework of the Gaussian process using a physically motivated feature space. The calculated average deviation and standard deviation are 0.046 MeV and 0.066 MeV, respectively. The results demonstrate that the binding energies are successfully modeled by the Gaussian process, reflecting the good learning ability of the Gaussian process in the calculations of binding energies. Then, we cal-

culate the binding energies for 108 nuclei, which are newly included in AME2020. The calculated results are in good agreement with the experimental data, which indicates the good predictive power of the Gaussian process in the studies of binding energies. Moreover, the application of the composite kernel function provides a novel perspective in studying other physical problems using the Gaussian process. Next, we calculate the α -decay energies due to the successful calculations of the binding energies using the Gaussian process. The average deviation and the standard deviation for 1169 nuclei with $50 \leq Z \leq 110$ are 0.047 MeV and 0.070 MeV, respectively. Notably, the theoretical α -decay energies for the new nuclides ^{204}Ac and ^{207}Th are well reproduced with $\Delta Q_\alpha = 0.0004$ MeV for ^{204}Ac and $\Delta Q_\alpha = 0.051$ MeV for ^{207}Th . The good results also show that the Gaussian process is reliable for the studies of binding energies. Finally, the α -decay properties for the actinide nuclei are predicted using the Gaussian process. We expect the predicted results will be useful for future studies of the binding energies and the α -decay properties.

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