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RESEARCH ARTICLE

Large-scale shell model calculation of neutron rich even-Even $^{54-66}\text{Fe}$ isotopes

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Abstract

Shell model calculations were performed to study the energy levels and the reduced transition probabilities $B(E2; 0_{g.s}^+ \rightarrow 2_1^+)$ for even-even $^{54-66}\text{Fe}$ neutron rich isotopes by using the shell model code Nushellx@MSU for windows by employing the effective interactions GXPF1, GXPF1A, KB3G and FPD6. The core is taken at ^{48}Ca for all nuclei under study and the results of our theoretical calculations for both energy levels and reduced transition probabilities $B(E2; 0_{g.s}^+ \rightarrow 2_1^+)$ are compared with the most recent available experimental data. A good agreement were obtained for all isotopes under study for energy levels and unable to reproduce the experimental data for the reduced transition probabilities using constant effective charges which proves the limitation of full-fp calculations.

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Introduction

The neutron rich nuclei in the *fp*-shell region are at the focus of attention of the nuclear physics community at present. Unstable nuclei in this region exhibit many new phenomenon such as appearance of new magic numbers and disappearance of well-established ones, softening of core at $N=28$, interplay of collective and single particle properties (Srivastava and Mehrotra, 2009). The 2^+ energy in these nuclei, and sometimes the 4^+ energy as well, could be well reproduced by shell-model calculations in which an *fp*-model space is employed. However, in the level sequences above the 4^+ states, structural changes have been observed in these systems that may require an inclusion of high-*j* orbitals in order to discuss these changes (Yang Sun et al., 2009).

It is a common feature of systems of interacting fermions to form a shell structure. In atomic nuclei the spin-orbit interaction lowers the energy of the orbitals with the highest angular momentum into the next lower oscillator shell with opposite parity, leading to the well-known sequence of magic numbers. While the shell structure and the resulting energy gaps between the orbitals explain many general properties of nuclei across the nuclear chart, it has become evident that the shell structure and magic numbers change for nuclei with large neutron excess. As protons and neutrons in such exotic nuclei occupy different orbitals compared to their stable counterparts, the effective single-particle energies are shifted. (Ljungvall et al., 2010).

Full *fp* -shell model study of $A=48$ nuclei were performed by Caurier and Zuker (Caurier and Zuker, 1994) by modifying Kuo-Brown (KB) (Kuo and Brown, 1968) to KB1 and KB3. The isobaric chains $A=50$, $A=51$ and $A=52$ studied by Poves et al. (Poves, et al. 2001) using KB3 and FPD6 (Richter et al., 1994) and their new released version KB3G.

Shell model study for full *fp*-shell model were performed by (Majeed and Auda, 2006) to study the levels schemes and transition rates $B(E2, \uparrow)$ for even-even $^{48-56}\text{Ti}$ isotopes by employing FPD6 and GXPF1 effective interactions.

Shell model calculations using Oxbash for windows (Brown, et al., 2004) by employing the residual effective interactions were performed to study the levels schemes and reduced transition probabilities for ^{46}Ti , ^{46}Cr and ^{46}V for the isovector $T=1$ positive parity states by (Majeed, 2008).

F. I. Sharrad (Sharrad, 2013) calculated the binding energies, energy levels and the reduced transition probabilities of neutron-rich $^{60-66}\text{Fe}$ isotopes by using Nushellx.

The aim of the present work is to study the reduced transition probabilities and level schemes of even-even $^{54-66}\text{Fe}$ isotopes using the shell model Nushellx for windows by employing the effective residual interactions fitted for the fp -shell region codenamed FPD6, GXPF1, GXPF1A and KB3G.

Shell model calculations

The calculation were carried out in the HO model space for nuclei even-even $^{54-66}\text{Fe}$ near the closed core ^{48}Ca by using Nushellx@MSU code for windows without any restriction imposed on the model space with four effective interactions codenamed GXPF1, GXPF1A, KB3G and FPD6 interactions. The calculation of excitation energy levels and reduced transition probabilities were compared with the most recent available experimental data and the best agreement achieved using **FPD6** effective interaction.

Within the framework of the shell model, an auxiliary one-body potential U is introduced in order to break up the Hamiltonian for a system of A nucleons as the sum of a one-body term H_0 , which describes the independent motion of the nucleons, and a residual interaction H_1 :

$$H = \sum_{i=1}^A \frac{p_i^2}{2m} + \sum_{i < j=1}^A V_{ij}^{NN} = T + V = (T + U) + (V - U) = H_0 + H_1 \dots \dots (1)$$

Once H_0 has been introduced, it is possible to define a reduced model space in terms of a finite subset of HO's eigenvectors. In this space, an effective Hamiltonian H_{eff} may be constructed and the diagonalization of the many-body Hamiltonian equation (1) in an infinite Hilbert space is then reduced to the solution of an eigenvalue problem in a finite space (Itaco, et al., 2011).

The reduced transition probability for electric multipole radiation is given by (Greiner and Maruhn, 1996)

$$B(E_l, J_i \rightarrow J_f) = \frac{2J_f + 1}{2J_i + 1} \left| \int d^3r \langle f | \hat{\rho}(r) r^l Y_l(\Omega) | f \rangle \right|^2 \dots \dots (2)$$

Where $\hat{\rho}(r)$: is the charge density operator

$Y_l(\Omega)$: is the spherical harmonics

Results and Discussion

The test of success of large-scale shell model calculations is the prediction of the first 2^+ level and the transition rates $B(E2; 0_{g.s}^+ \rightarrow 2_1^+)$ using the optimized effective interactions for the description of fp -shell nuclei (Majeed and Auda, 2006) For all isotopes under investigation the core are taken at ^{48}Ca and the valence nucleons distributed over $1f_{7/2}$, $2p_{3/2}$, $1f_{5/2}$ and $2p_{1/2}$ orbits.

Energy levels

Figure 1 presents the comparison between our theoretical calculations for the energy levels using the residual effective interactions FPD6, GXPF1, GXPF1A and KB3G with the experimental data taken from Ref. (ENSDF, 2014). Good agreement were obtained for all interactions employed in the present work and the best results achieved by employing FPD6 effective interaction.

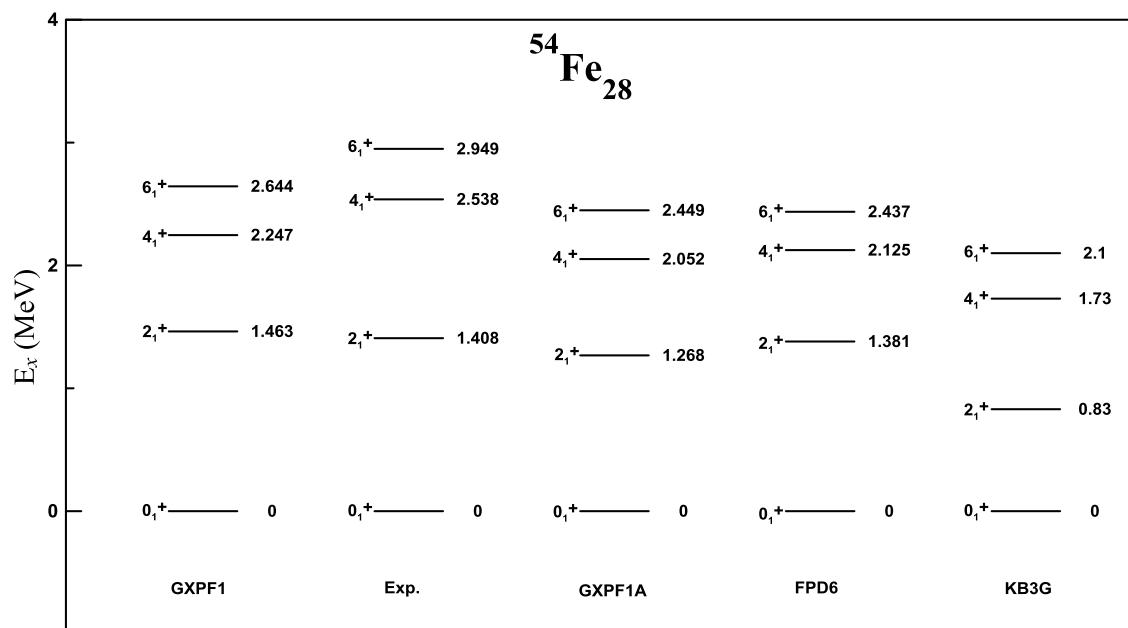


FIG. 1: Comparison of the experimental excitation energies taken from Ref. (ENSDF, 2014) with the present theoretical work using FPD6, GXPFF1,GXPFF1A and KB3G effective interactions for ^{54}Fe nucleus.

A comparison between our theoretical works by employing the four effective interactions mentioned in the present work with the recent experimental data for the isotopes ^{56}Fe and ^{58}Fe is shown in Figures 2 and 3. In general there is good global agreement with the experimental data and the best results achieved for both isotopes by GXPFF1A effective interaction.

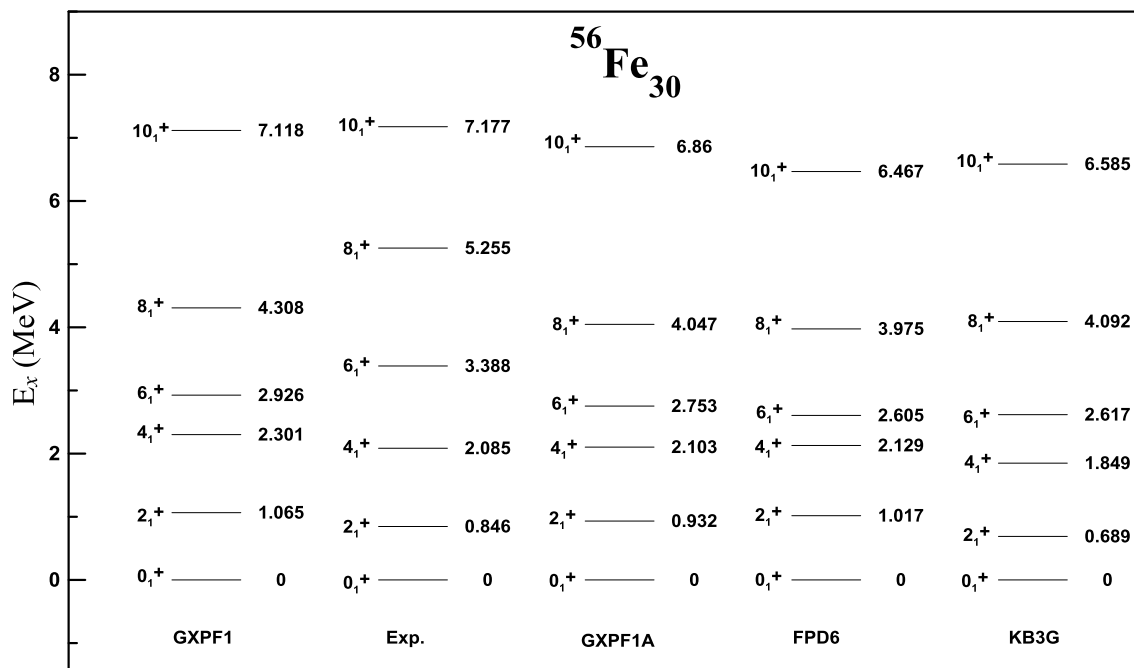


FIG. 2: Comparison of the experimental excitation energies taken from Ref. (ENSDF, 2014) with the present theoretical work using FPD6, GXPFF1,GXPFF1A and KB3G effective interactions ^{56}Fe nucleus.

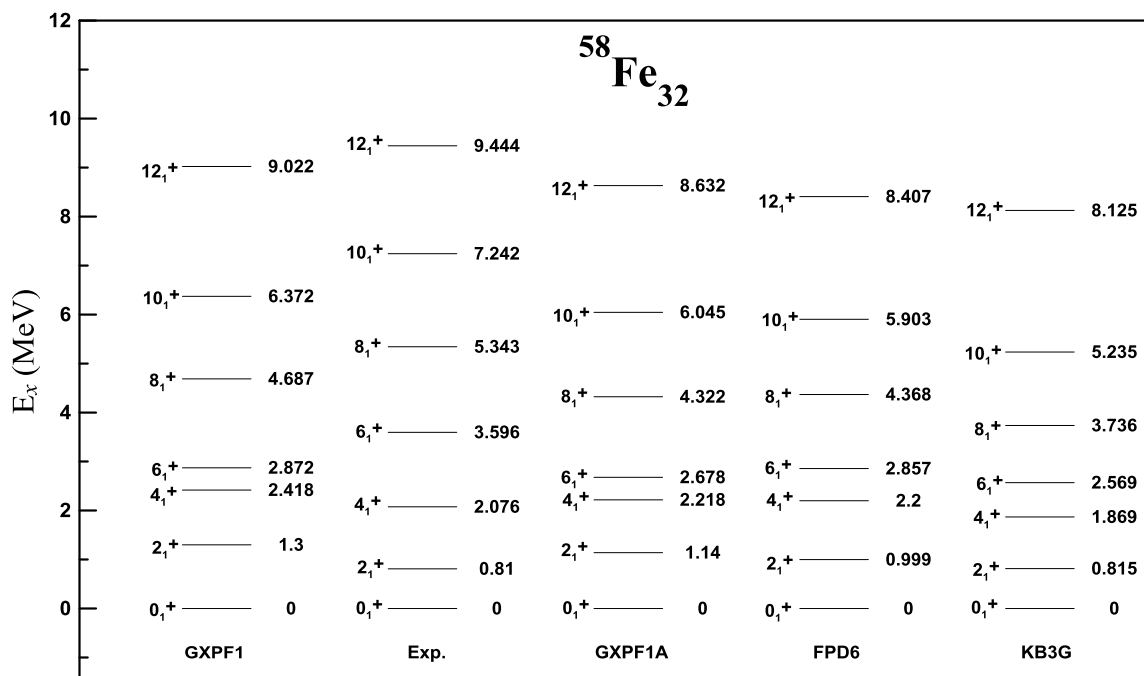


FIG. 3: Comparison of the experimental excitation energies taken from Ref. (ENSDF, 2014) with the present theoretical work using FPD6, GXPF1, GXPF1A and KB3G effective interactions ^{58}Fe nucleus.

Same comparison were also presented in figures 4, 5, 6 and 7 and the best results were obtained by using GXPF1A and FPD6 effective interactions.

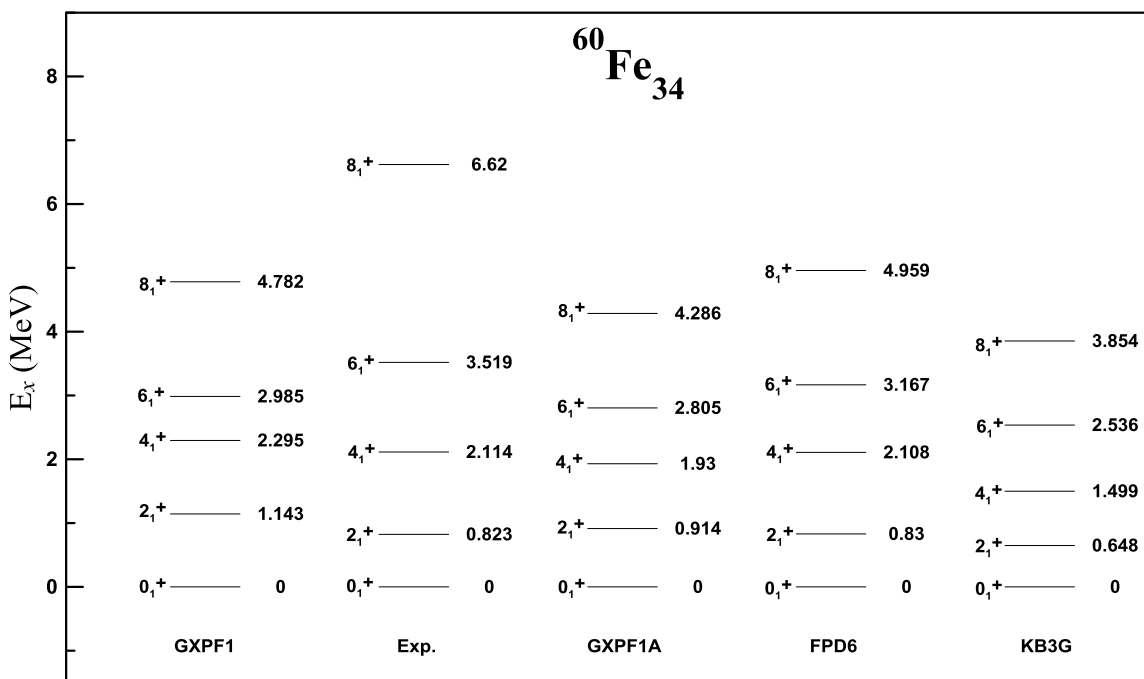


FIG.4: Comparison of the experimental excitation energies taken from Ref. (ENSDF, 2014) with the present theoretical work using FPD6, GXPF1, GXPF1A and KB3G effective interactions ^{60}Fe nucleus.

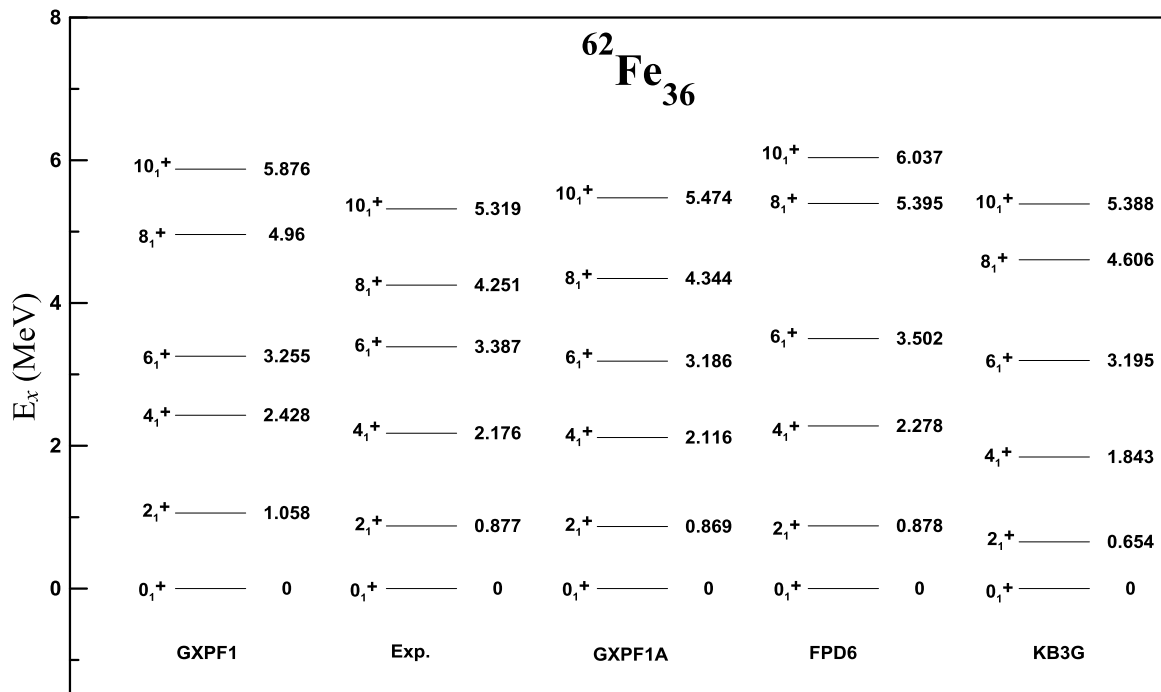


FIG. 5: Comparison of the experimental excitation energies taken from Ref. (ENSDF, 2014) with the present theoretical work using FPD6, GXPF1,GXPF1A and KB3G effective interactions ^{62}Fe nucleus.

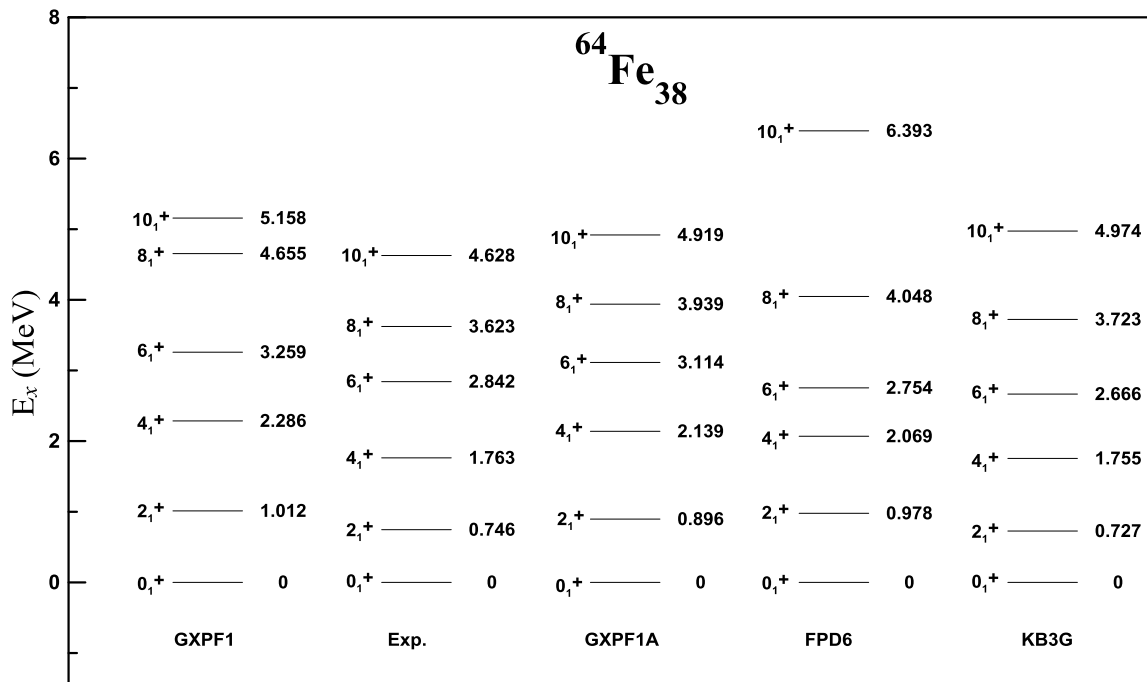


FIG. 6: Comparison of the experimental excitation energies taken from Ref. (ENSDF, 2014) with the present theoretical work using FPD6, GXPF1,GXPF1A and KB3G effective interactions ^{64}Fe nucleus.

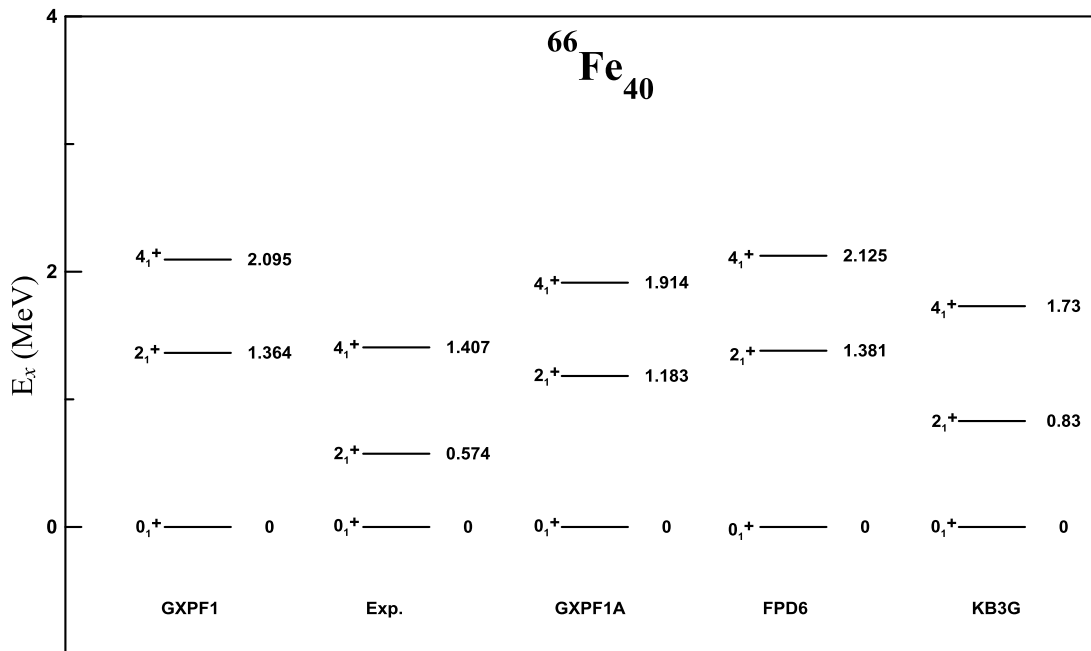


FIG. 7: Comparison of the experimental excitation energies taken from Ref. (ENSDF, 2014) with the present theoretical work using FPD6, GXPF1, GXPF1A and KB3G effective interactions ^{66}Fe nucleus.

Figure 8, presents a systematic comparison for the first 2^+ and 4^+ energy levels with their corresponding experimental values. From the comparison it is evident that the best effective interaction is FPD6 that describe these isotopes lies in the fp -shell region.

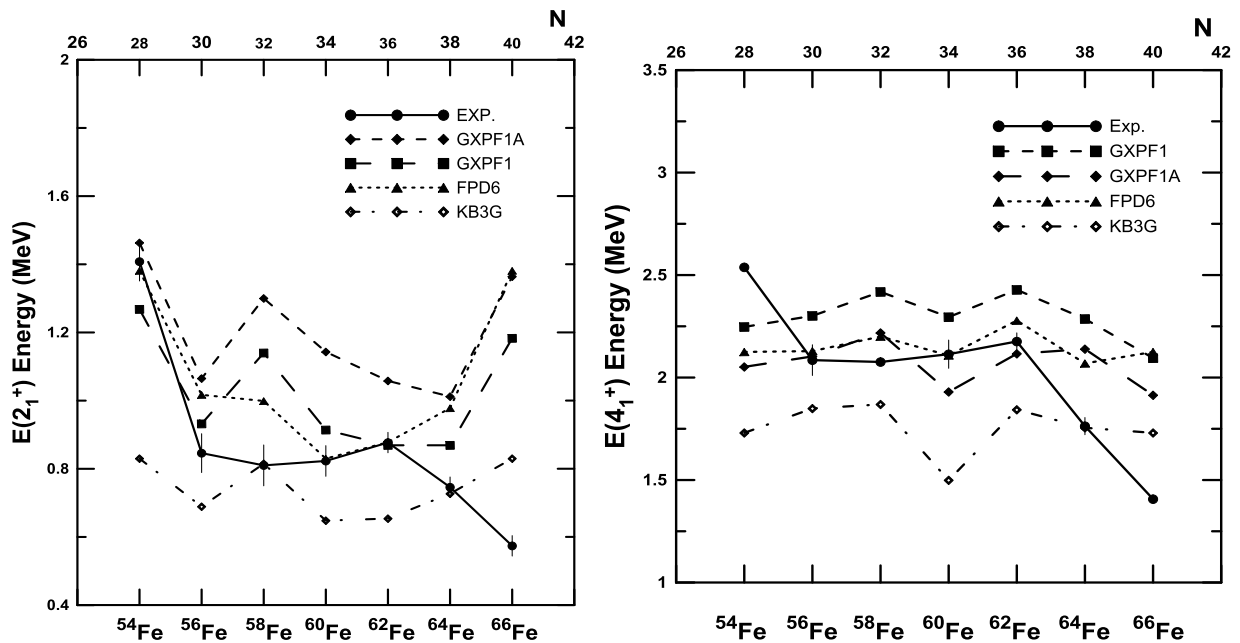


FIG. 8: Systematics of $E_x(2_1^+)$ and $E_x(4_1^+)$ for even-even Fe isotopes. Experimental data (filled circles) [ENSDF, 2014] are compared with present by employing FPD6, GXPF1, GXPF1A and K3BG effective interactions.

Transition probabilities

Since the transition rates represent a sensitive test for the most modern effective interactions that have been developed to describe *fp*-shell nuclei. The transition strengths calculated in this work performed using the harmonic oscillator potential HO for each in-band transition by assuming pure E2 transition. The effective charges were taken to be $e_{\pi}=1.25e$ for proton and $e_{\nu}=0.8e$ for neutron.

Figure 9 presents the comparison between the calculated reduced transition probabilities for all isotopes using FPD6 effective interaction with the experimental data. From the figure it is shown that there is agreement only for the isotopes ^{54}Fe and ^{56}Fe and the calculations starts to deviate severely for the rest of the isotopes due to increase of the number of valence neutrons which effect the structure evolution of these isotopes and effect the theoretical prediction of these isotopes.

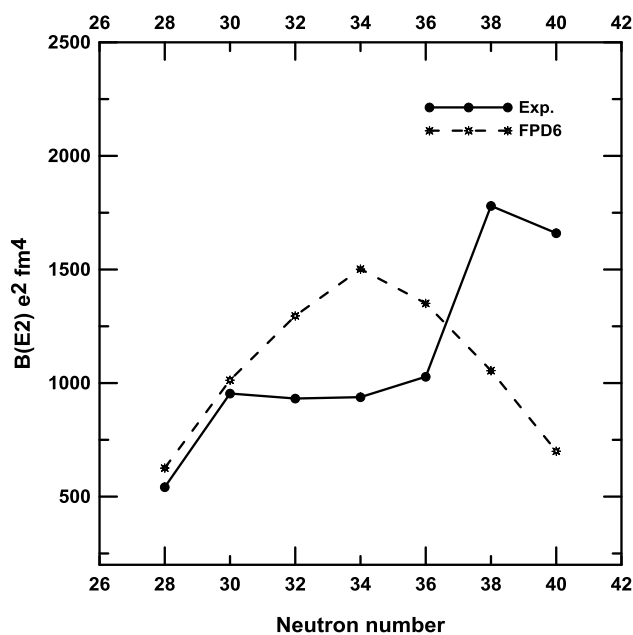


FIG.9: Comparison of the large-scale shell model calculations using FPD6 (stars) with the experimental $B(E2; 0_{g.s}^+ \rightarrow 2_1^+)$ transition strengths (closed circles) [NNDC, 2014] for the chain of even-even Fe isotopes.

Conclusions

The present study demonstrated that the best effective interactions that might be used to describe nuclei lies in the *fp*-shell region is FPD6 and GXPF1A. The use of constant effective charges for the proton and neutron are not always the best choice to describe the dynamic properties of the nuclei such as the reduced transition probabilities $B(E2)$, especially when the neutron number increase that effect the structure evolution of the nuclei with neutron rich access. This work can be extended to study more neutron rich chain of isotopes to have better understanding of these effective interactions and the possible ways to modify them to be more agreeable with the experimental data.

Acknowledgments

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