

Superheavy Elements in Kilonovae

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ABSTRACT

As LIGO-Virgo-KAGRA enters its fourth observing run, a new opportunity to search for electromagnetic counterparts of compact object mergers will also begin. The light curves and spectra from the first “kilonova” associated with a binary neutron star binary (NSM) suggests that these sites are hosts of the rapid neutron capture (“*r*”) process. However, it is unknown just how robust elemental production can be in mergers. Identifying signposts of the production of particular nuclei is critical for fully understanding merger-driven heavy-element synthesis. In this study, we investigate the properties of very neutron rich nuclei for which superheavy elements ($Z \geq 104$) can be produced in NSMs and whether they can similarly imprint a unique signature on kilonova light-curve evolution. A superheavy-element signature in kilonovae represents a route to establishing a lower limit on heavy-element production in NSMs as well as possibly being the first evidence of superheavy element synthesis in nature. Favorable NSMs conditions yield a mass fraction of superheavy-elements is $X_{Z \geq 104} \approx 3 \times 10^{-2}$ at 7.5 hours post-merger. With this mass fraction of superheavy elements, we find that kilonova light curves may appear similar to those arising from lanthanide-poor ejecta. Therefore, photometric characterizations of superheavy-element rich kilonova may possibly misidentify them as lanthanide-poor events.

Keywords: Nucleosynthesis (1131), R-process (1324), Light curves (918), Nuclear astrophysics (1129), Nuclear fission (2323), Nuclear decay (2227), Compact objects (288)

1. INTRODUCTION

The joint multi-messenger detection of gravitational waves and electromagnetic emission from the merger of two neutron stars in 2017 (Abbott et al. 2017a) represented a new opportunity for observational studies of heavy-element production. Sixty years after the *r*-process was first theorized (Burbidge et al. 1957; Cameron 1957), the NSM event GW170817 (Abbott et al. 2017b) and its corresponding afterglow AT2017gfo

(Coulter et al. 2017; Cowperthwaite et al. 2017; Drout et al. 2017; Kilpatrick et al. 2017; Shappee et al. 2017) provided the first direct evidence that binary neutron star mergers can host the *r*-process (Kasen et al. 2017; Smartt et al. 2017; Tanaka et al. 2017; Tanvir et al. 2017; Villar et al. 2017; Watson et al. 2019), supporting a theory proposed decades earlier (Lattimer & Schramm 1974). Consequently, recent studies of compact object mergers and *r*-process nucleosynthesis have focused on macrophysical and microphysical properties that can be deduced from compact object merger light curves, e.g., broad parameter estimation of ejecta masses and velocities (Coughlin et al. 2019; Radice & Dai 2019; Breschi et al. 2021; Heinzel et al. 2021). In addition, fission,

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which was known to be a critical factor in determining the abundance pattern, e.g. [Beun et al. \(2008\)](#); [Vassh et al. \(2020\)](#), was now realized to be an important predictor of the light curve. Recent studies have investigated the detailed elemental compositions of the ejecta and fission properties of heavy nuclei ([Wu et al. 2019](#); [Vieira et al. 2023](#)). In general, composition inference and the claim that r -process elements were synthesized in the GW170817 event are based on the effect of high-opacity lanthanides ($57 \leq Z \leq 71$) on the light-curve evolution, and it cannot currently be definitively claimed that anything beyond the lanthanides were created in that event, see [Zhu et al. \(2018\)](#).

Recent works have detailed the effects of ejecta mass and composition on kilonova light curves ([Barnes et al. 2021](#); [Zhu et al. 2021](#); [Lund et al. 2023](#)) and have even identified an individual nucleus that can power the light curve at late times: ^{254}Cf ([Zhu et al. 2018](#)). With a half life of about 60 days, the energy released by the spontaneous fission of ^{254}Cf , can prolong the evolution of light in the JHK bands, leaving a measurable excess of light beginning as early as 25 days post-merger. Such a late-time detection would be observational proof that the actinides ($89 \leq Z \leq 103$) are synthesized in mergers—not just the lanthanides. Other works have also discussed individual nuclei that can power the late-time light curves (e.g., [Wu et al. 2019](#)).

An earlier signal could possibly arise from the energetic decay of even heavier nuclei: the “superheavy” elements with $Z \geq 104$. Whether these elements are even produced by nature is a topic of debate and depends sensitively on the nuclear physics at high proton and neutron numbers ([Holmbeck et al. 2023](#)). In this work, we explore a subset of nuclear models that can produce superheavy elements in an NSM environment and study the effect that superheavy elements have on kilonova light curves.

2. NUCLEOSYNTHESIS OF SUPERHEAVY ELEMENTS

To investigate the effect of superheavy elements on kilonova light curves, we first choose conditions that favorably produce these elements. Across r -process nucleosynthesis studies, see ([Arcones & Thielemann 2023](#)) and references therein, it is found that conditions that generally produce high actinide abundances are the low-entropy and high neutron-richness of dynamical ejecta from NSMs. Therefore, we choose a single dynamical ejecta trajectory from the $1.4\text{--}1.4M_{\odot}$ NSM simulations of S. Rosswog ([Piran et al. 2013](#); [Rosswog et al. 2013](#)) as in [Korobkin et al. \(2012\)](#). We run nucleosynthesis simulations with the nuclear reaction network code

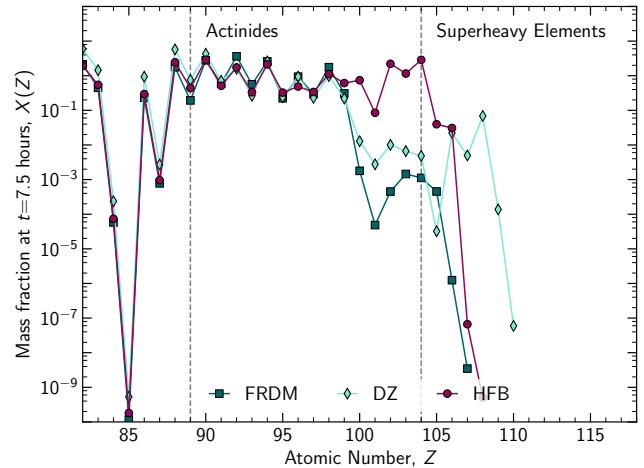


Figure 1. Nucleosynthesis network mass-fraction yields of the heaviest elements at 7.5 hours post-merger for three nuclear mass model and fission barrier combinations. Under the same astrophysical conditions, there can be over three orders of magnitude difference in the mass fractions of superheavy elements that are synthesized, arising solely from what nuclear models are adopted.

Portable Routines for Integrated nucleoSynthesis Modeling (PRISM; [Sprouse 2020](#)) and begin the network in nuclear statistical equilibrium at 10 GK.

Even under the most favorable environmental conditions (low-entropy and high neutron-richness), superheavy-element production is not guaranteed. Specifically, low fission barriers can cause heavy nuclei to fission before superheavy elements can be produced (see, e.g., [Mumpower et al. 2018](#); [Vassh et al. 2019](#)). To investigate the range of superheavy-element production that can be achieved by different nuclear models, we test three nuclear model and fission barrier combinations: the Finite Range Liquid Droplet Model (FRLDM; [Möller et al. 2015](#)) for the 2012 version of the Finite Range Droplet Model (FRDM; [Möller et al. 2012, 2016](#)), fission barriers based on the Koura-Tachibana-Uno-Yamada model (KTUY [Koura et al. 2005](#)) for Dufo-Zuker (DZ; [Dufo & Zuker 1995](#)), and Hartree-Fock-Bogoliubov (HFB; [Goriely et al. 2007](#)) for HFB (version 27; [Goriely et al. 2013](#)). Experimentally measured data are used wherever possible in all nucleosynthesis calculations, regardless of the other choice of theoretical model. Otherwise, reaction and decay rates are calculated as self-consistently as possible with the given nuclear model (or experimentally measured mass, if available) and fission barrier heights as in [Mumpower et al. \(2015\)](#).

We use the same astrophysical conditions for all three cases. As the composition evolves over time, nuclear reheating from the decay of radioactive species affects the

temperature evolution of the trajectory. The reaction rates are in turn affected by the temperature change relative to the original trajectory. Since the energy released by radioactive nuclei depends on nuclear mass differences, the reheating calculation is performed to be consistent with the specific theoretical (and experiment) nuclear masses implemented. We adjust the temperature of the trajectory from nuclear reheating self-consistently with the nuclear physics input to determine the extent to which the temperature evolution needs modification and recalculate reaction rates accordingly.

Figure 1 shows the heavy-element mass fractions at 7.5 hours post-merger for three nuclear variations. The HFB model has the highest mass fraction of superheavy elements at this time, concentrated primarily at $Z = 104$ (Rf). FRDM is among the most pessimistic, producing superheavy elements of about four orders of magnitude less than the actinides, while DZ achieves significant mass fractions as heavy as $Z = 108$ (Hs), though in overall less amounts than HFB. For this study, we will choose the two extremes, FRDM and HFB, to examine the effect that superheavy elements have on NSM light curves. At 7.5 hours, the mass fractions of lanthanides, actinides, and superheavy elements for FRDM (HFB) are $X_{\text{lan}} = 0.094$ (0.10), $X_{\text{act}} = 0.14$ (0.18), and $X_{Z \geq 104} = 1.6 \times 10^{-5}$ (3.0×10^{-2}), respectively.

3. LIGHT CURVE CALCULATION

The two most basic ingredients to translate abundance evolution into light curves are heating (including thermalization effects) and ejecta opacities. First, as radioactive nuclei made in the r -process decay, they release energy, a fraction of which is converted to thermal photons (“thermalized”), which ultimately power the kilonova’s electromagnetic emission.

3.1. Heating rates

The output of PRISM, along with the underlying nuclear data—both experimental and calculated—are used to determine the rate at which heat is generated by the ejecta as well as its composition over time, as in [Zhu et al. \(2021\)](#). We calculate light curves representing three different levels of contribution from heavy-element decay. First we calculate heating rates and light curves for all nuclei from the PRISM output (“ $Z = \text{all}$ ”). Secondly, as a simple test, we remove the effects $Z \geq 104$ nuclei (the superheavy elements) from the heating-rate calculation (“ $Z < 104$ ”). In other words, any reaction or decay involving $Z \geq 104$ elements is assumed to contribute zero energy, but we do not otherwise remove the nuclei from the network calculation. Lastly, we mute the effects of all $Z \geq 90$ nuclei on the heating rate calcula-

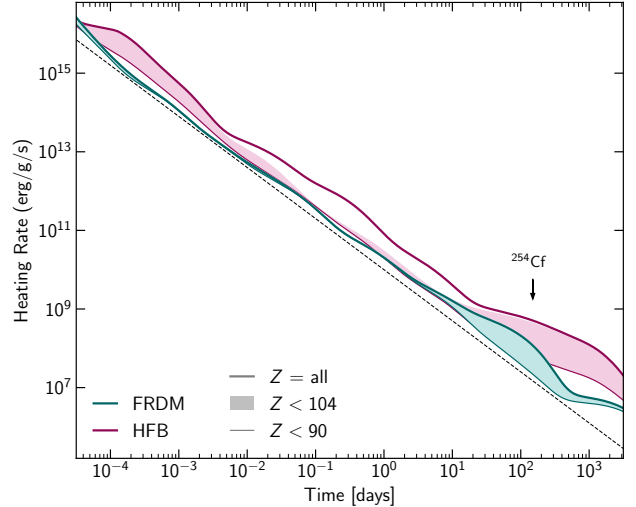


Figure 2. Heating rates over time for two extremes of nuclear variations showing the contribution by all elements (thick, solid lines), only up to the actinides (shaded), and excluding the actinides and superheavy elements (thin, solid lines). The dashed line is a simple model in which the heating rate evolves scales with time by $10^{-1.3}$ (see, e.g., [Metzger 2019](#)). The divergence between the shaded region and the thick lines (e.g., at about 10^{-2} – 10^1 days for HFB) indicates heating uniquely from the superheavy elements.

tion, such that only $Z \leq 89$ elements impact the heating of the system (“ $Z < 90$ ”).

For the sake of studying the direct effect that superheavy elements have on kilonova light curves, we use an identical astrophysical environment (which is subject to nuclear-model-dependent reheating from actinides and superheavy elements) and alter the heating rate post-facto, as described above, though we note that a more complex approach is necessary to account for the indirect effects that superheavy elements would have on the light curve, e.g., through the decay of their fission products at lower atomic masses. We expect that removing both the direct and indirect products of superheavy elements would only further differentiate the heating rate, and thus our approach provides a lower bound.

Figure 2 shows the total heating rates for the three nuclear models for three different cases: with only $Z < 90$ nuclei (thin lines), only $Z < 104$ nuclei (filled), and all nuclei (solid lines). Going from the thin lines to the top of the filled regions shows the direct effect that actinides have on the heating rates. Notably, both models show a dramatic increase at about 100 days due to the spontaneous fission of ^{254}Cf ([Zhu et al. 2018](#)). The differences between the top of the filled regions and the solid lines show the unique effect that superheavies have on the heating rates, differentiable from the actinides.

For FRDM, there is no apparent difference between the “ $Z = \text{all}$ ” and “ $Z < 104$ ” cases owing to FRDM producing very small mass fraction of superheavy elements (see Figure 1). With the HFB model, several discernible features appear on time scales ranging from about 0.2 hours out to several days. Two of the most prominent superheavy-unique features appear at approximately seven hours ($10^{-0.5}$ days) and several days ($10^{0.4}$ days) post-merger.

The first feature in the heating rate at about seven hours is primarily due to the spontaneous fission of odd- A nuclei with $Z = 104\text{--}106$ and $N = 169\text{--}171$. The cause of this spontaneous fission dominance is two-fold; first, the abundance of material that is able to reach this region is due to the high fission barriers (i.e., lower fission probabilities) associated with the HFB model (Vassh et al. 2019). This effect is apparent in Figure 1, which shows, for example, the mass fraction of $Z = 104$ isotopes that is several orders of magnitude larger in HFB than in the results from the FRDM calculation. Secondly, the probabilities for nuclei to decay by fission, β , or α differ between FRDM and HFB, therefore affecting both the energy and time scales predicted between the two models.

The second peak in the HFB “ $Z = \text{all}$ ” heating rate at a few days post-merger also largely stems from the spontaneous fission of $^{270,271}\text{Rf}$. Again, we attribute this to both the build-up of material at $Z = 104$ as well as the theoretical rates (and, therefore, branching ratios) differing between FRDM and HFB that contribute to the population of these nuclei. In the next section, we investigate how this signature in the heating rate manifests as an observational signature in the light curve.

3.2. Thermalization and radiation transport

To calculate light curves, we use both the PRISM composition and the predicted fraction of the radioactive energy released by α -decay, β -decay, and fission (the relevant decay processes on kilonova timescales). With the energy partitioned by decay channel, we employ analytic estimates of particle-specific thermalization efficiencies (Kasen & Barnes 2019) following Zhu et al. (2021) to derive the rate at which thermal energy is imparted to the kilonova ejecta as a function of time. This approach means that the difference in the thermalization rates of our models are due solely to differences in the relative importance of α -decay, β -decay, and fission; we do not carry out a full calculation of particle emission and propagation (though see Barnes et al. 2021, for a detailed discussion of self-consistent thermalization simulations).

In addition to different heating rates, the three variations we study here also have different compositions, which affects the light curves by altering the ejecta opacity. When specifying the composition for each variant, we remove the indicated elements (i.e., actinides and superheavies, actinides only, or no elements) and renormalize the resulting composition so the mass fractions of the remaining elements sum to unity.

The calculation of the opacity depends on the atomic structure of the elements in the ejecta. Specifically, due to the periodicity of the periodic table, the atomic structure of elements is a function primarily of the block in the table that it occupies, and secondarily on its position within its row (Kasen et al. 2013; Tanaka & Hotokezaka 2013; Tanaka et al. 2020).

Because we lack synthetic atomic data for the full set of elements synthesized by the r -process, we use a simplified composition in our radiation transport simulations. As f -block elements, lanthanides and actinides supply most of the opacity, and the kilonova emission is most sensitive to their total mass fraction and abundance pattern. We take the lanthanide and actinide abundances from PRISM (or from the modified PRISM outputs), and modify them only to account for our lack of atomic data for $Z = 72$ and the actinide species. The abundance predicted for $Z = 72$ is assigned to $Z = 71$ in our proxy composition. Additionally, the abundance predicted for each actinide element is assigned to the lanthanide that occupies the same position in the periodic table row, e.g., lanthanum is a proxy for actinium. We model the contribution of d -block elements by summing their mass fractions and dividing the total evenly among $21 \leq Z \leq 28$. The remaining mass is assigned to $Z = 20$, which acts as a low-opacity filler. On the periodic table, the superheavy elements with $104 \leq Z \leq 112$ occupy the d -block, and will therefore contribute as lower-opacity elements. The detailed radiation transport is then calculated with *Sedona* (Kasen et al. 2006; Roth & Kasen 2015) as in Barnes et al. (2021), assuming a spherically symmetric outflow with variable ejecta mass (see Section 3.4) and an average ejecta velocity $v/c = 0.1$.

3.3. Light curves

Figure 3 shows the bolometric light curves for two nuclear cases (FRDM and HFB) with the three heating-rate variations. For all cases in Figure 3, we assume an ejecta mass of $0.005 M_{\odot}$. The gray curves show the light curve with only $Z < 90$ nuclei, that is, without any actinides or superheavy elements directly contributing to the heating rate. The dotted colored curves show the light curve when actinides are allowed to contribute to the total heating; i.e., heating is from all nuclei with

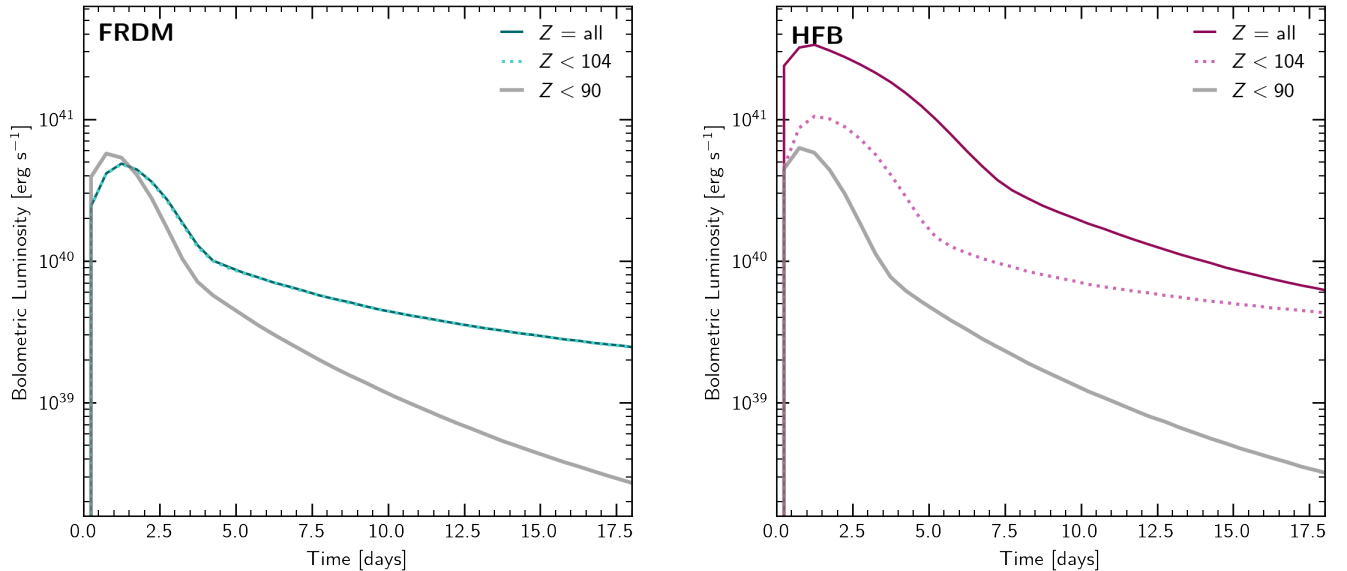


Figure 3. Bolometric light curves using the FRDM nuclear model (left) and the HFB model (right) assuming an ejecta mass of $0.005 M_{\odot}$. For each nuclear model, three sets of heating rates are used: only $Z < 90$ elements (solid gray), only $Z < 104$ elements (dotted colors), and all elements (solid colors). The paucity of superheavy elements produced in the FRDM simulation explains why the green solid (“ Z =all”) and light-blue dotted (“ $Z < 104$ ”) curves appear identical; there is effectively no difference between these models.

$Z < 104$. Already differences arise compared to the no-actinide case. First more energy is radiated over the course of the light curve. For FRDM, this manifests on the light-curve tail, which is much brighter when actinides are included in the heating. For HFB, both the peak and the tail of the “ $Z < 104$ ” light curve are more luminous than for the “ $Z < 90$ ” case. Regardless of nuclear mass model, the light curve declines more slowly when actinides are present. Second, the added opacity of the actinides also broadens the light curve, delaying the peak relative to models without actinides. The solid, colored curves in Figure 3 show the bolometric luminosity achieved when all nuclei (including the superheavies) participate in the heating. For FRDM, the effect is negligible, owing to the paucity of superheavy elements that are produced when using FRDM fission barriers (see Figure 1). However, the higher fission barrier heights of HFB14 allow significant superheavy-element production, dramatically increasing the brightness and overall duration of the light curve.

Under the same astrophysical conditions—not only in thermodynamic evolution, but also in ejecta mass and velocity—the superheavy elements can leave a distinct signature on the light curve that is unique from the actinides. If an event were to display such an evolution of its light, not only would it be the first observational evidence that superheavy elements are produced astrophysically, but it would also help constrain the unknown nu-

clear physics by placing limits on fission barrier heights of neutron-rich nuclei.

3.4. Observationally differentiating superheavy-element production

While the superheavy element signature is evident in Figure 3, when observing kilonovae we do not know the ejecta mass a priori. The question remains whether there is a discernible signature of superheavy-element production in light curves that have similar time-dependent bolometric luminosities. To explore this idea, we adjust the ejecta masses for each case such that the total heating rates at one day are equal to the FRDM “ $Z = \text{all}$ ” case with $0.005 M_{\odot}$ (see Figure 3). This normalization produces light curves of similar bolometric luminosities. The HFB ejecta masses required to produce the desired heating rates are 0.00051 , 0.00163 , and $0.00541 M_{\odot}$ for the “ $Z = \text{all}$,” “ $Z < 104$,” and “ $Z < 90$ ” cases, respectively. With these normalized ejecta masses, we recalculate the bolometric luminosities.

Figure 4 shows the results for HFB when the ejecta masses are renormalized, corresponding to the case in which the light curves are roughly the same brightness at about one day. Because the overall contribution of the actinides and superheavies is decreased (by virtue of lowering the total ejecta masses in those cases), their effects on the light curve are significantly less than in Figure 3, in which identical ejecta masses were used for each light curve calculation. Notably, the inclusion of

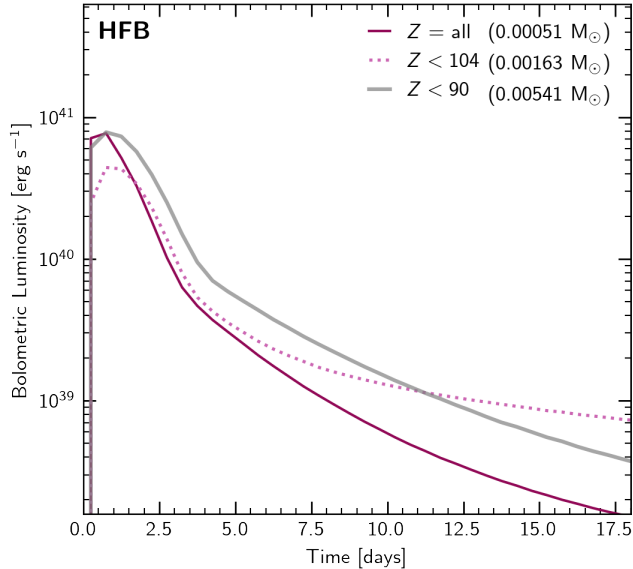


Figure 4. Bolometric light curves for the HFB model (right) with ejecta es renormalized such that the heating rates at one day is equal for all models. Three sets of heating rates: only $Z < 90$ elements (gray), only $Z < 104$ elements (dashed pink), and all elements (dark pink).

actinides produces a light curve with a slightly fainter luminosity at peak and a slower-decaying evolution at late times (longer than five days). However, if the composition includes the superheavies in addition to the actinides, the effect on the late-time light curve diminishes. In addition, within the first few days, the light curve decays much more quickly (note how the dark pink peak is narrower than the other cases).

This effect arises both from the effective redistribution (between mass models) of the composition from high-opacity elements into low-opacity ones as well as the quick decay of those elements. The superheavies act as additional d -block elements, optically similar to the iron-peak elements that could be expected to form in lower neutron-richness environments (such as an accretion disk wind), despite requiring a very high neutron flux in order to synthesize them. This effect may be exacerbated by the excess heat from the decay of the superheavy elements, which can produce low-opacity ionization states in the ejecta at early times (Tanaka et al. 2020; Barnes et al. 2021).

Figure 5 shows the broad band light curves in the normalized-mass case for both the FRDM and the HFB calculations in which the full range of elements are allowed to contribute to the heating rate. Here we treat the FRDM calculation as the case in which superheavy elements are not present in the ejecta rather than manually removing the superheavy elements from the HFB

calculation. Differences in these two light curves highlight the unique effects—both direct and indirect—that superheavy (and not just actinide) elements have on the kilonova light curve evolution. The presence of actinides and lanthanides (and their associated heating) in the FRDM case leads to late-time emission in the red bands, while the fast and energetic decays of the superheavy elements in the HFB case lead to earlier, brighter emission in the blue bands. However, neither start as blue-band bright as AT2017gfo. Note that actinides are still present in the HFB calculation, and we stress that a component containing superheavy elements should be considered in light curve models. For example, the AT2017gfo data is commonly fit with two components (see, e.g., Cowperthwaite et al. 2017): a “blue” (low opacity) and a “red” (high opacity). A superheavy-element component in our investigation acts like an additional blue component in composition, despite containing high-opacity elements. Further studies should explore whether the AT2017gfo data shows evidence for a separate, superheavy-element-containing component.

4. CONCLUSION

In this study, we have explored and selected a combination of nuclear data and astrophysical conditions that allows production of superheavy elements in order to examine their potential impact on observables (i.e., kilonova light curves). So far, no evidence of the natural production of $Z \geq 104$ elements has been definitively found (though see claims of superheavy decay products found in meteorites; references in Holmbeck et al. 2023). If superheavy elements have a unique effect on light curves, it may be possible to infer their production in NSMs. Such an identification would be the first observational evidence of superheavy elements being synthesized by nature. This possibility is the motivation behind the present analysis.

First, we achieved superheavy-element production by using the nuclear masses and fission barrier heights of the HFB model and the neutron-rich tidal tails of NSM ejecta. We find that superheavy elements can lead to light curves that decline quickly after peak brightness and continue to fall through the following weeks post-merger. This rapid decline is in conflict with the extended late-time emission that the presence of lanthanides and actinides has on kilonova ejecta. In addition, ejecta that includes actinides and superheavy elements produces a light curve similar in evolution to a ten-times-as-massive actinide-free event. Our results demonstrate another natural degeneracy between NSM ejecta composition and mass, this time due to the pres-

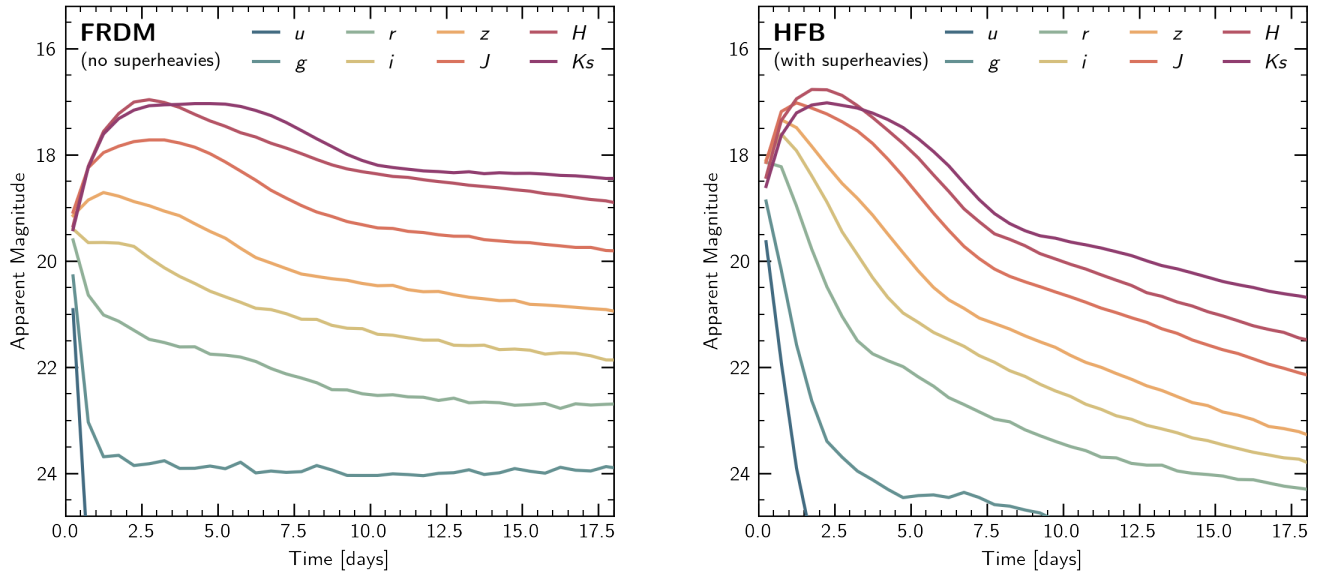


Figure 5. The effect of superheavy elements on broad-band light curves for the full FRDM (no superheavy elements) and HFB (with superheavy elements) under similar observational conditions (lines).

ence (or lack) of superheavy elements in the merger ejecta.

We have only considered spherically symmetric outflows by the neutron-rich tidal ejecta in this work since those conditions can favorably produce the superheavy elements. A lanthanide-poor component could plausibly produce similar broad-band light curves, further increasing the degeneracy between ejecta mass and composition. Furthermore, the lack of an extended light curve does not rule out the presence of actinides in merger ejecta, and care should be taken when deriving lanthanide mass-fractions from kilonova observations. If there is a degeneracy in the light curve evolution—a photometric quantity—then one possibility that remains to be explored is whether the superheavy elements are distinguishable spectroscopically. Such a study would require extensive atomic physics dedicated to characterizing the features that could be visible in kilonova spectra.

The way in which superheavies contribute to the total heating rate of NSM ejecta depends on fission rates at high atomic mass numbers. Therefore, the possibility of the astrophysical production of superheavy elements is still contingent on as-of-yet theoretical nuclear data. Advances in nuclear theory and experiment will be able to uncover whether, e.g., fission suppresses superheavy-element production in NSMs.

With the possibility of more observational light curves accompanying NSM candidates detected by the next gravitational wave observing run, we have the new opportunity to observe—for the first time—superheavy-element formation as it occurs. However, there is a

growing need to resolve discrepancies and degeneracies from nuclear and astrophysics modeling before definitive conclusions about elemental production are drawn from kilonova observations.

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