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On the Elusive Twelfth Vibrational State of Beryllium Dimer

Konrad Patkowski *et al.*

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details). We explored the tidal stripping effects at a spatial resolution (~100 pc) several times as high as that of typical simulations of galaxy clusters, checking 32 different orbital configurations. We converted the stellar density maps produced by our simulations into surface brightness and processed them using the SExtractor software in the same way as we did for the search of cE galaxies in HST images.

Our simulations demonstrate the efficiency of tidal stripping in reducing the stellar mass of a disc galaxy. Even in cases of quasicircular orbital configurations, the large-scale stellar disc was heavily stripped, decreasing the galaxy stellar mass by a factor of 2 (Fig. 3) on a time-scale of 600 to 700 million years. We compared the evolution of total magnitude, surface brightness, and internal velocity dispersion of a stripped galaxy to observations (Fig. 1, top and middle). Interactions on radial orbits resulted in heavier mass loss of up to 90%, although a remnant became quickly accreted by a cD galaxy. Presumably, by scaling down the systems in mass, that is, by replacing a giant disc with a low-luminosity or dwarf S0, it should be possible to reproduce the formation of UCD and transitional cE/UCD (*28*, *11*) galaxies.

In our study, we used Virtual Observatory data mining to reclassify cE galaxies from "unique" to "common in certain environmental conditions," that is, more frequent than was previously thought. We confirmed the nature of 21 galaxies selected by the VO workflow with follow-up observations and archival data. We also reproduced their properties with numerical simulations. We can confirm that tidal stripping of the stellar component plays an important role in the morphological transformation of galaxies in dense environments, producing remnants spanning a luminosity range of four orders of magnitude.

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13. VizieR Catalogue Service; http://vizier.u-strasbg.fr
14. NASA/IPAC Extragalactic Database; http://nedwww.ipac.caltech.edu
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32. This study is based on observations made with the NASA/European Space Agency (ESA) Hubble Space Telescope and obtained from the Hubble Legacy Archive, which is a collaboration between the Space Telescope Science Institute (NASA), the Space Telescope European Coordinating Facility (ESA), and the Canadian Astronomy Data Centre (National Research Council Canada/Canadian Space Agency); observations collected with the 6-m telescope of the Special Astrophysical Observatory of the Russian Academy of Sciences operated under the financial support of the Science Department of Russia (registration number 01-43). The simulations were run on the Callisto cluster at the École Polytechnique Fédérale de Lausanne and on the Regor cluster of the Geneva Observatory. This research made use of SAOImage DS9, developed by Smithsonian Astrophysical Observatory; Aladin, developed by the Centre de Données Astronomiques de Strasbourg (CDS), "exploresdss" script by G. Mamon; the VizieR Catalogue access tool (CDS); and the NASA/IPAC Extragalactic Database (NED) operated by the Jet Propulsion Laboratory, California Institute of Technology, under contract with NASA. Funding for the SDSS and SDSS-II has been provided by the Alfred P. Sloan Foundation, the participating institutions, the National Science Foundation, the U.S. Department of Energy, NASA, the Japanese Monbukagakusho, the Max Planck Society, and the Higher Education Funding Council for England. The SDSS Web site is www.sdss.org. The simulation data analysis and galaxy maps were done using the parallelized Python pNbody package (http://obswww.unige.ch/~revaz/pNbody). This work was supported by the Swiss National Science Foundation.
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Figs. S1 to S3
Tables S1 and S2
References

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On the Elusive Twelfth Vibrational State of Beryllium Dimer

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The beryllium dimer has puzzled chemists for roughly 80 years on account of its unexpectedly strong bonding interaction between two nominally closed-shell atoms. Recent spectroscopic measurements characterized the molecule's ground electronic state with sufficient resolution to distinguish 11 vibrational levels; the possibility that a twelfth level lay just below the dissociation threshold remained unresolved. Here we present a potential function, based on ab initio calculations at the full configuration interaction level, that definitively supports the presence of this twelfth vibrational state. "Morphed" versions of this potential, fitted to experimental data, closely reproduce the observed spectra to within 0.1 cm^{-1}, bolstering the strength of the assignment.

Merritt *et al.* (*1*) recently reported a spectroscopic study of the beryllium dimer, an unusual diatomic system that is bound by about 2.5 kcal/mol and has an equilibrium interatomic separation of 2.44 Å. This bond is within the range of van der Waals interactions, but is substantially stronger and shorter than those between other similarly sized closed-shell atoms. Spectroscopic measurements for Be_2 are difficult to perform, and the experiment (*1*) resulted in a markedly altered prediction of the well depth for the ground electronic state: from $D_e = 790 \pm 30$ cm^{-1} (*2*, *3*) to 929.7 ± 2.0 cm^{-1} (*1*). The study also increased the number of identified vibrational levels from 5 to 11. The authors suspected that one more level could exist, but their empirical fit to the measured data predicted only 11 levels, with the vibrational quantum number v ranging from 0 to 10. The existence of a twelfth level, bound by a fraction of a wavenumber,

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would provide information about the shape of the potential at large interatomic separations R and could be relevant to experiments on ultracold trapped atoms (*4*). We show here that the $v = 11$ state can be positively identified from ab initio calculations.

Because Be_2 is a fairly small system (only eight electrons), it has been one of the benchmarks for computational ab initio methods, with more than 100 studies published [see (*5*, *6*) for lists of references]. The calculations are nonetheless difficult due to the *sp* near-degeneracy of the atomic orbitals of beryllium (*6*). This near-degeneracy, which is the reason that Be_2 is more strongly bound than He_2 or Ne_2, results in poor performance of standard electron correlation methods based on single-determinant reference functions. Recent calculations using methods beyond a single-determinant reference consistently gave a well depth significantly deeper than the earlier experimental prediction (*2*, *3*). In particular, the most extensive calculations gave a depth of 938 ± 15 cm^{-1} (*6*), several standard deviations beyond the experimental result up to that point. Thus, the measurement of Merritt *et al*. (*1*) reconciled experiment with theory and provided another example of the predictive power of modern ab initio methods.

Our group has been working for some time on extending the single-point calculations of (*6*) to other interatomic separations. As in (*6*), the interaction energies were constructed here from contributions at several levels of theory up to the frozen-core full configuration interaction method. The effects beyond the frozen-core approximation and relativistic effects were also included. All the calculations used the largest basis sets that exist for Be or that can be currently applied at a given level of theory within reasonable computer resource constraints, and were extrapolated to complete basis set limits. An analysis of the patterns of convergence with the level of theory and size of the basis sets provided estimated uncertainties $\sigma(R)$ of the results. The ab initio interaction energies computed for 20 interatomic separations were fitted by an analytic function of a form often used for van der Waals interactions of atoms:

$$V_{\mathrm{vdW}}(R) = (A + BR + C/R + DR^2 + ER^3) \times e^{-\alpha R + \beta R^2} - \sum_{n=3}^{8} f_{2n}(bR)\frac{C_{2n}}{R^{2n}} \qquad (1)$$

where $f_n(bR)$ are the Tang-Toennies damping functions (*7*),

$$f_n(bR) = 1 - \mathrm{e}^{-bR}\sum_{m=0}^{n}(bR)^m/m! \qquad (2)$$

C_n are the asymptotic coefficients (*8*) that were kept constant during the fitting process, and the parameters α, β, b, A, B, C, D, and E were obtained in a nonlinear least-squares fitting procedure with the ab initio results weighted according to their uncertainties $\sigma(R)$. The unweighted root-mean square error (rmse) of the fit is 0.78 cm^{-1}. The values of the fit parameters are given in table S1.

The fit was used to compute rovibrational levels of Be_2, and the results are presented in Table 1. Our purely ab initio potential function V_{vdW} recovers the measured vibrational energies (column "Exp.") with rmse of only 3.4 cm^{-1}, a substantial improvement over the previous best ab initio predictions (*9*–*12*), and furthermore predicts the existence of the $v = 11$ state 0.52 cm^{-1} below the dissociation limit. Merritt *et al*. found a spectral feature quite close to this position [marked by an arrow in Fig. 1 of (*1*)], which they attributed to the onset of the continuum, but which could correspond to the twelfth state. We have also computed the transition intensities for the stimulated emission pumping spectrum recorded in (*1*) (fig. S1) and found that the transition to $v = 11$ should be strong enough to observe.

Our ab initio potential predicts a well 9 cm^{-1} deeper than the empirical potential of Merritt *et al*. To rule out the possibility that this discrepancy might account for the emergence of the $v = 11$ level in the calculation, we generated two additional analytic potentials V_+ and V_-. These potentials share the functional form and the asymptotic

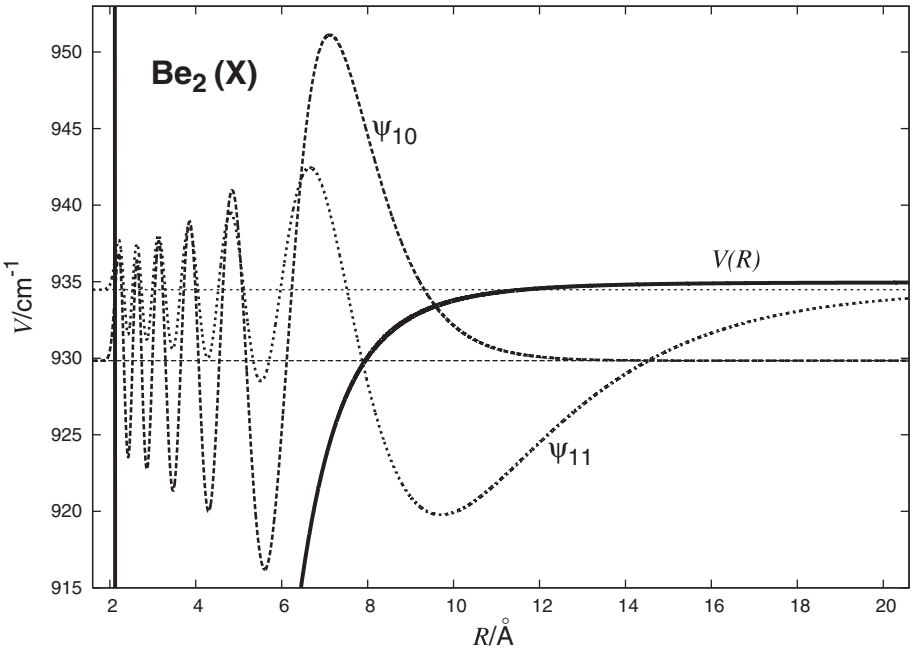

Fig. 1. The calculated wave functions of the $v = 10$ and $v = 11$ vibrational states of the ground electronic state of Be_2. The dashed horizontal lines are the positions of the two states.

Table 1. Comparison of spectra predicted by empirical, ab initio, and morphed potentials with experiment. The energy unit is cm^{-1} and the equilibrium distances R_e are given in Å. The Δ columns present the difference between the values in the preceding column and the experimental values [Exp., from (*1*)]. Emp. refers to the empirical potential in (*1*), V_{vdW} to the ab initio potential, $\tilde{V}^{(2)}_{\mathrm{vdW}}$ to the two-parameter morphed potential of Eq. 3 (with $a = 0.99390732$ and $b = 1.00215597$), and $\tilde{V}^{\mathrm{RPC}(3)}_{\mathrm{vdW}}$ and $\tilde{V}^{\mathrm{RPC}(5)}_{\mathrm{vdW}}$ to the potential morphed according to three- and five-parameter RPC algorithms, respectively.

v	Exp.	Emp.	Δ	V_{vdW}	Δ	$\tilde{V}^{(2)}_{\mathrm{vdW}}$	Δ	$\tilde{V}^{\mathrm{RPC}(3)}_{\mathrm{vdW}}$	Δ	$\tilde{V}^{\mathrm{RPC}(5)}_{\mathrm{vdW}}$	Δ
1	222.6	222.7	0.1	222.3	−0.3	221.9	−0.7	221.9	−0.7	222.6	0.0
2	397.1	397.8	0.7	397.6	0.5	396.4	−0.7	396.4	−0.7	397.0	−0.1
3	518.1	518.2	0.1	520.3	2.2	518.2	0.1	518.2	0.1	518.2	0.1
4	594.8	595.4	0.6	597.9	3.1	595.1	0.3	595.1	0.3	594.8	0.0
5	651.5	652.4	0.9	655.1	3.6	652.0	0.5	651.9	0.4	651.5	0.0
6	698.8	699.4	0.6	702.6	3.8	699.2	0.4	699.1	0.3	698.7	−0.1
7	737.7	738.2	0.5	741.7	4.0	738.0	0.3	737.9	0.2	737.6	−0.1
8	768.2	768.8	0.6	772.4	4.2	768.3	0.1	768.2	0.0	768.2	0.0
9	789.9	790.7	0.8	794.3	4.4	789.7	−0.2	789.7	−0.2	790.0	0.1
10	802.6	803.4	0.8	807.1	4.5	802.0	−0.6	802.1	−0.5	802.5	−0.1
11*				811.9	(0.52)	806.4	(0.41)	806.6	(0.44)	807.1	(0.42)
rmse			0.6		3.4		0.4		0.4		< 0.1
D_e		929.7		938.7		933.0		933.2		934.6	
R_e		2.454		2.443		2.438		2.432		2.438	

*The number in parentheses is the separation between the $v = 11$ state and the onset of the continuum. The empirical potential does not support the $v = 11$ bound state.

constants with V_{vdW}, but are fitted to reproduce the values of $E_{int} + \sigma$ and $E_{int} - \sigma$, respectively, instead of the ab initio interaction energies E_{int}. Both V_+ and V_- support the $v = 11$ state, which lies at respective frequencies 0.38 and 0.70 cm^{-1} below the onset of the continuum. Because the minimum depth of V_+ is 922.1 cm^{-1} (i.e., 8 cm^{-1} shallower than the empirical potential), the well depth is clearly not a determining factor in the appearance of the $v = 11$ state.

The ab initio potential reproduces measured transitions with errors about six times larger than the empirical potential of (*1*). To find out if a closer recovery of the transitions does not lead to disappearance of the $v = 11$ level, we developed a semi-empirical, "morphed" form of V_{vdW}. In the morphing process, the ab initio potential is fine-tuned by introducing a small number (up to five in this work) of adjustable parameters with values fitted to experimental data. The simplest form of morphing is a variation of the energy and length scales in the potential

$$\tilde{V}^{(2)}_{vdW}(R) = aV_{vdW}(bR) \qquad (3)$$

via two fitted scaling factors *a*,*b*. The second approach (*8*), an extended version (*13*, *14*) of the reduced potential curve (RPC) method proposed by Jenč and Plíva (*15*), can be viewed as a more general form of scaling. The experimental data points used in the morphing procedure were the vibrational energies and rotational transitions. The fit and the RPC morphing parameters are given in tables S1 and S2.

The predictions of our three morphed potentials are compared with experimental values in Table 1. All show better agreement with measured data than the empirical potential obtained by Merritt *et al.* (*1*). Moreover, there is an order of magnitude improvement relative to the predictions of our ab initio potential, which was distorted to an only minor extent by the morphing (shown by the values of D_e and R_e). All morphed potentials predict the existence of the $v = 11$ level at a position 0.41 to 0.44 cm^{-1} below the dissociation limit, in good agreement with the purely ab initio value. The $v = 11$ vibrational state is not only bound, but supports two excited rotational states.

The failure of the fit of Merritt *et al.* (*1*) to predict the $v = 11$ state can be attributed mainly to its poor asymptotic behavior. Our ab initio calculations were performed for *R* up to 8 Å, and we used nearly exact van der Waals constants in our fit. Thus, the long-*R* portion of our fit is very accurate. Merritt *et al.* used a purely exponential form of the fit, which has an unphysical decay at large *R*. Indeed, the discrepancies of this fit relative to V_{vdW} are up to 2.4 cm^{-1} in the 5 to 8 Å range where the interaction potential ranges between −87 and −5 cm^{-1}. This region is critical for the high-*v* states, as shown in Fig. 1. The vibrational wave function of the $v = 11$ state has a maximum magnitude around 10 Å. Because this wave function is mainly sensitive to the region of the potential well approximated by the asymptotic $-C_6/R^6$ term, one can use the semi-classical near-dissociation theory of Le Roy and Bernstein (*16*) to determine the number of bound levels. If the experimental dissociation energies of the $v = 9$ and $v = 10$ states are used as input, this theory predicts that there exists one more bound vibrational state above these two. It is gratifying to see that the simple qualitative picture of the near-dissociation theory agrees with our quantitative ab initio description of vibrational levels in the beryllium dimer.

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SOM Text
Fig. S1
Tables S1 and S2
References

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From Hydrogenases to Noble Metal–Free Catalytic Nanomaterials for H_2 Production and Uptake

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Interconversion of water and hydrogen in unitized regenerative fuel cells is a promising energy storage framework for smoothing out the temporal fluctuations of solar and wind power. However, replacement of presently available platinum catalysts by lower-cost and more abundant materials is a requisite for this technology to become economically viable. Here, we show that the covalent attachment of a nickel bisdiphosphine–based mimic of the active site of hydrogenase enzymes onto multiwalled carbon nanotubes results in a high–surface area cathode material with high catalytic activity under the strongly acidic conditions required in proton exchange membrane technology. Hydrogen evolves from aqueous sulfuric acid solution with very low overvoltages (20 millivolts), and the catalyst exhibits exceptional stability (more than 100,000 turnovers). The same catalyst is also very efficient for hydrogen oxidation in this environment, exhibiting current densities similar to those observed for hydrogenase-based materials.

One dilemma inherent in the widespread use of solar cells and windmills for power generation is that temporal fluctuations in worldwide energy demand do not strictly correlate with the availability of sunlight and wind. An efficient, reversible means of storing excess energy is necessary, and unitized regenerative fuel cells are an attractive option for that purpose. The devices operate by storing energy in hydrogen generated via electrolysis of water and then releasing it as necessary through the reverse reaction. The devices are compact and have low internal resistance. However, they currently rely on platinum for catalysis, which is too scarce and thus too expensive for widespread adoption (*1*). A competitive alternative may be found in microorganisms that metabolize hydrogen using hydrogenase enzymes (*2*, *3*). These metalloproteins bidirectionally catalyze interconversion between H_2 and a pair of protons and electrons (the same

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