Precise Predictions of Charmed-Bottom Hadrons from Lattice QCD

Nilmani Mathur,[1,*] M. Padmanath,[2,†] and Sourav Mondal[1]
[1]*Department of Theoretical Physics, Tata Institute of Fundamental Research, Homi Bhabha Road, Mumbai 400005, India*
[2]*Institüt für Theoretische Physik, Universität Regensburg, Universitätsstrase 31, 93053 Regensburg, Germany*

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We report the ground state masses of hadrons containing at least one charm and one bottom quark using lattice quantum chromodynamics. These include mesons with spin (J) and parity (P), (J^P): 0^-, 1^-, 1^+, and 0^+ and the spin 1/2 and 3/2 baryons. Among these hadrons, only the ground state of 0^- is known experimentally, and therefore our predictions provide important information for the experimental discovery of all other hadrons with these quark contents.

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Recently, heavy hadron physics has attracted huge scientific interest mainly due to the prospects of studying new physics beyond the Standard Model at the intensity frontier [1–5] and to study various newly discovered subatomic particles to better understand the confining nature of strong interactions [6–12]. From the perspective of newly found hadrons itself, a large number of discoveries over the past decade ranging from the usual mesons [13–20] and baryons [21] along with their excited states [22–25] to new exotic particles like tetraquarks [26–28] and pentaquarks [29], as well as hadrons whose structures are still elusive [6–8,30–33], have proliferated interest in the study of heavy hadrons. Furthermore, it is envisaged that the large data already collected or to be obtained at different laboratories, particularly at LHCb and Belle II, will further unravel many other hadrons. One variety of such theorized but as yet essentially unobserved (except one) subatomic particles are hadrons made of at least a charm and a bottom quark, the charmed-bottom (bc) hadrons.

Investigations of such hadrons are highly appealing, as they provide a unique laboratory to explore the heavy quark dynamics at multiple scales: $1/m_b$, $1/m_c$, and $1/\Lambda_{\rm QCD}$. Decay constants and form factors of bc mesons are still unknown but are quite important because of their relevance to investigate physics beyond the Standard Model, particularly in view of the recent measurement of $R(J/\psi)$ [34]. The information on spin splittings and decay constants can shed light on their structures and help us to understand the nature of strong interactions at multiple scales. Moreover, bc baryon decays can aid in studying the $b \to c$ transition and $|V_{cb}|$ element of the Cabibbo-Kobayashi-Maskawa matrix.

However, to date, the discovery of these hadrons is limited to only two observations: $B_c(0^-)$ with mass 6275(1) MeV [35] and $B_c(2S)(0^-)$ at 6842(6) MeV [36], while the latter has not yet been confirmed [37]. On the other hand, the LHC being an efficient factory for producing bc hadrons [38,39], one would envisage their discovery and study their decays in the near future. Precise theoretical predictions related to the energy spectra and decay of these hadrons are thus utmost essential to guide their discovery.

In fact, various model calculations exist in the literature on bc mesons [40–46] and baryons [47–53]. However, those predictions vary widely; e.g., $1S$-hyperfine splitting in $B_c(\bar{b}c)$ mesons spread over a range of 40–90 MeV [40–46]. The predictions on bc baryons and excited states are even more scattered. Naturally, first-principles calculations using lattice QCD are quite essential to study these hadrons. However, unlike quarkonia, lattice study of bc hadrons is confined only to a few calculations [54–58]. In this work, we carry out a detailed lattice calculation of the ground state energy spectra of all low-lying bc hadrons (shown in Table I) with very good control over systematics and predict their masses most precisely to this date.

Lattice QCD studies are subject to various lattice artifacts. Of these, the most relevant one in a study of heavy hadrons is the discretization error. It is thus essential to take a controlled continuum extrapolation of the results from finite lattice spacings. To that goal, we obtain results at three lattice spacings: $a \sim 0.12$, 0.09, and 0.06 fm and then are able to perform such extrapolations. Below, we elaborate our numerical procedure.

Numerical details: A. Lattice ensembles.—We use three dynamical $2+1+1$ flavors (u/d, s, and c) lattice ensembles generated by the MILC Collaboration [59] with highly improved staggered quark (HISQ) fermion action [60]. The lattices are with sizes $24^3 \times 64$, $32^3 \times 96$, and $48^3 \times 96$ at gauge couplings $10/g^2 = 6.00$, 6.30, and 6.72, respectively

TABLE I. List of bc hadrons that we study in this work. Quantum numbers (J^P) along with the valence quark contents are also mentioned.

Mesons ($\bar{q}_1 q_2$)	Baryons ($[q_1 q_2 q_3](J^P)$) $J^P \equiv 1/2^+$	$1/2^+$	$3/2^+$
$B_c(\bar{b}c)(0^-)$	$\Xi_{cb}[cbu]$	$\Xi'_{cb}[cbu]$	$\Xi^*_{cb}[cbu]$
$B^*_c(\bar{b}c)(1^-)$	$\Omega_{cb}[cbs]$	$\Omega'_{cb}[cbs]$	$\Omega^*_{cb}[cbs]$
$B_c(\bar{b}c)(0^+)$	$\Omega_{ccb}[ccb]$		$\Omega^*_{ccb}[ccb]$
$B_c(\bar{b}c)(1^+)$	$\Omega_{cbb}[bbc]$		$\Omega^*_{cbb}[bbc]$

[59]. The measured lattice spacings, obtained from the r_1 parameter, for the set of ensembles being used here are 0.1207(11), 0.0888(8), and 0.0582(5) fm, respectively [59].

B. Quark actions.—For valence quark propagators, from light to charm quarks, we use the overlap action which has exact chiral symmetry at finite lattice spacings [61–63] and no $\mathcal{O}(ma)$ error. A wall source is utilized for calculating quark propagators.

For the bottom quark, we utilize a nonrelativistic QCD (NRQCD) formulation [64] in which we incorporate all terms up to the leading term of the order of $1/M_0^3$, where $M_0 = am_b$ is the bottom mass [65,66]. This Hamiltonian is improved by including spin-independent terms through $\mathcal{O}(\alpha_s v^4)$ with nonperturbatively tuned improvement coefficients [67]. For the coarser two ensembles, we study the spectrum using *"improved"* coefficients as well as tree-level coefficients (*"unimproved"*).

C. Quark mass tuning.—Following the Fermilab prescription for heavy quarks [68], we tune the heavy quark masses by equating the spin-averaged kinetic mass of the $1S$ quarkonia states $[\bar{M}_{\rm kin}(1S) = \frac{3}{4}M_{\rm kin}(1^-) + \frac{1}{4}M_{\rm kin}(0^-)]$ to their physical values [66,69]. A momentum-induced wall source, which is found to be very efficient compared to point or smeared sources [70], is utilized to obtain kinetic masses precisely. The tuned bare charm quark masses are found to be 0.528, 0.427, and 0.290 on coarse to fine lattices, respectively, which also satisfy $m_c a \ll 1$, a necessary condition for reducing discretization effects. We tune the strange quark mass, following Ref. [71].

D. Hadron interpolators.—For mesons, we utilize the local meson interpolators ($\bar{b}\Gamma c$), where Γ, corresponding to different spin (J) and parity (P) quantum numbers J^P, are $\gamma_5(0^-)$, $\gamma_i(1^-)$, $I(0^+)$, and $\gamma_5\gamma_i(1^+)$. We work with the assumption that the extracted ground state with $\gamma_5\gamma_i$ is 1^+ and is unaffected by a possible nearby 2^+ level [54]. For baryons, we utilize the conventional interpolators given by $P^+[(q_1^T C\Gamma q_2)q_3]$ as discussed in detail in Refs. [57,58,72]. For spin-1/2 Ξ_{cb} and Ω_{cb}, $\Gamma = \gamma_5$, whereas for spin-1/2 Ξ'_{cb}, Ω'_{cb} and spin-3/2 Ξ^*_{cb}, Ω^*_{cb} we use $\Gamma = \gamma_i$ ($i = 1, 2, 3$) with appropriate spin projections. A subtlety in the Ξ_{cb}' correlators is the possible admixture of Ξ_{cb} baryons. However, the use of a wall source helps us to clearly distinguish these two correlators, which suggests that these two correlators coupled to two distinct states with no significant admixture. In the heavy quark limit, the total spin of the bc diquark becomes a good quantum number, and thus the mixing is heavily suppressed. An agreement between our results on these baryons with those obtained in Ref. [57] also justifies this observation. Below, we elaborate our results.

Results.—To cancel out the bare quark mass term which enters additively into the NRQCD Hamiltonian, we calculate the mass differences between energy levels rather than masses directly. To obtain the mass of a hadron (M_H^c), we first calculate subtracted masses on the lattice as

$$\Delta M_H = [M_H^L - n_b\overline{1S}_b/2 - n_c\overline{1S}_c/2]a^{-1}, \tag{1}$$

where $\overline{1S}_b$ and $\overline{1S}_c$ are the lattice calculated spin-average $\overline{1S}$ bottomonia and charmonia masses, respectively, whereas n_b and n_c are the number of b and c valence quarks, respectively, in the hadron. After calculating this subtracted mass, we perform the continuum extrapolation to get its continuum value ΔM_H^c. Finally, the physical result is obtained by adding the physical values of spin-average masses to ΔM_H^c as

$$M_H^c = \Delta M_H^c + n_b(\overline{1S}_b)_{\rm phys}/2 + n_c(\overline{1S}_c)_{\rm phys}/2. \tag{2}$$

Since the $B_c(0^-)$ mass is known experimentally, we also utilize a dimensionless ratio,

$$R_H = \frac{M_H^L - n_b\overline{1S}_b/2}{M^L_{B_c(0^-)} - n_b\overline{1S}_b/2}, \tag{3}$$

which is then extrapolated to the continuum limit (R_H^c), and the final hadron mass is obtained from

$$M_H^c = R_H^c \times (M_{B_c(0^-)} - n_b\overline{1S}_b/2)_{\rm phys} + n_b(\overline{1S}_b)_{\rm phys}/2. \tag{4}$$

These procedures of utilizing dimensionless ratios as well as mass differences for the continuum extrapolations substantially reduce the systematic errors arising from mass tuning as well as for the terms which enter masses additively. We used both Eqs. (2) and (4) and found consistent results and added the difference in systematics. Below, we discuss results for bc mesons and baryons.

Mesons.—In Fig. 1, we plot the subtracted mass (ΔM_H), as defined in Eq. (1), for $B_c(0^-)$ as a function of lattice spacings (a). Blue circles represent unimproved and red squares represent improved results. We extrapolate unimproved results using fit forms $Q^f = A + a^2 B$ as well as $C^f = A + a^3 B$. Two bands corresponds to one sigma error for these fittings (purple, Q^f; green, C^f). The extrapolated result and the experimental value are shown by red and blue

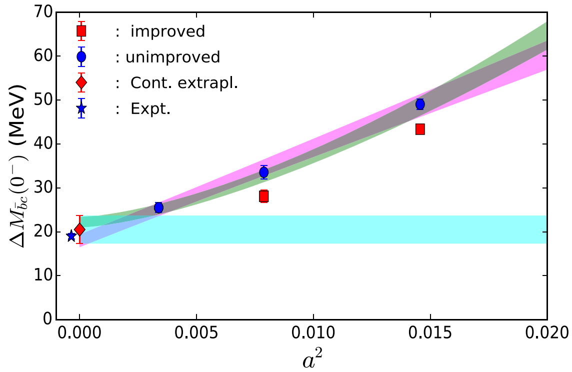

FIG. 1. Ground state mass of the $B_c(0^-)$ meson at three lattice spacings is shown in terms of energy splittings from the spin-average mass [Eq. (1)]. Continuum extrapolated and experimental values are also shown.

stars, respectively. As expected, the improved results are closer to the continuum limit (horizontal cyan bands show the proximity of the improved results from the continuum result). To see the consistency in fits, we also use a constrained fit with both forms together by loosely constraining A values from previous fits, and differences in fitted parameters are included in the discretization error. As in Fig. 1, throughout we follow the same conventions for symbols and color coding. In Fig. 2(top), we plot the hyperfine splitting of $1S$ B_c mesons. After the continuum extrapolation, we obtain $B_c^*(1^-) - B_c(0^-) = 55(3)$ MeV,

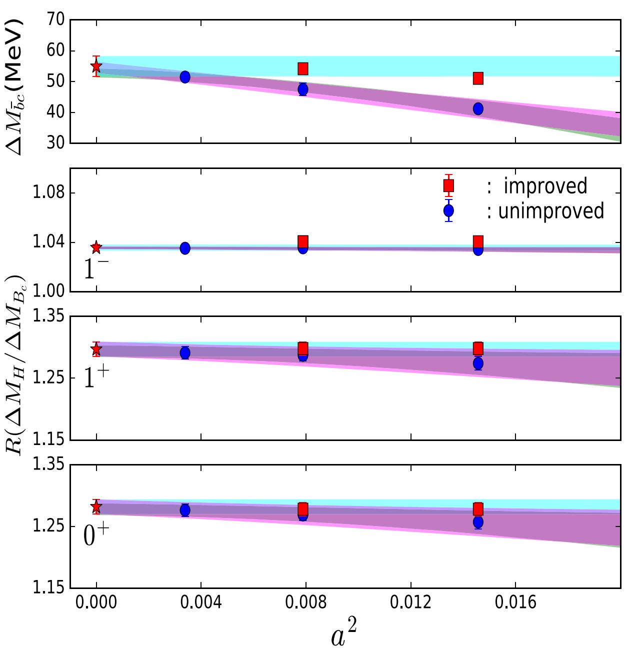

FIG. 2. (Top) Hyperfine splitting in B_c mesons at three different lattice spacings and at the continuum limit. (Bottom three) Ratios [as defined in Eq. (5)] of subtracted masses of 1^-, 1^+, and 0^+ mesons to that of the 0^- B_c meson are plotted at three lattice spacings and at the continuum limit.

which is consistent with previous lattice calculations [54,56] but more precise. In the bottom figure, we show the subtracted ratios [Eq. (3)] and continuum extrapolations for the ground states of 1^-, 1^+, and 0^+ B_c mesons. Taking the experimental values for $B_c(0^-)$ and $1\bar{S}$ quarkonia [35] masses, we obtain the ground state masses for these mesons and tabulate those in Table II.

Baryons.—We first discuss the Ξ_{cb} baryons. The presence of a valence light quark in Ξ_{cb} demands a chiral extrapolation. The use of a multimass algorithm allows us to simulate a range of pion masses. In Fig. 3(top), we plot Ξ_{cb} masses at various pion masses which clearly show a quadratic variation starting from the physical pion mass to ~600 MeV. We thus use a chiral extrapolation of the form $A + m_\pi^2 B$. Within the limit of acceptable χ^2/dof, variations in chiral extrapolation forms, as in Ref. [57], do not change the final value. The same procedure is repeated for Ξ'_{cb} and Ξ^*_{cb} at three lattices. These chiral extrapolated values are then used to calculate the subtracted masses and are plotted in the bottom part in Fig. 3. These subtracted masses are then extrapolated to the continuum limit to get the ground state masses of these baryons and are tabulated in Table II. In Fig. 4, we show lattice extracted ΔM_H and the continuum extrapolations for different Ω baryons with flavor content bcs, bcc, and bbc, respectively. Continuum extrapolated results are shown by stars in each figure and are listed in Table II.

Error estimation.—Below, we address the estimation of various errors related to this work.

Statistical.—The use of a wall source reduces the statistical errors substantially and facilitates wide and stable fit ranges even for baryons. We find that the statistical error is always below the percent level and is maximum for the Ξ_{cb} baryons, which is about 0.4%.

TABLE II. Ground state masses of B_c mesons and baryons as predicted in this work. Statistical and systematic errors are shown inside two parentheses, respectively.

Hadrons	Lattice	Experiment
$B_c(0^-)$	6276(3)(6)	6274.9(8)
$B_c^*(1^-)$	6331(4)(6)	?
$B_c(0^+)$	6712(18)(7)	?
$B_c(1^+)$	6736(17)(7)	?
$\Xi_{cb}(cbu)(1/2^+)$	6945(22)(14)	?
$\Xi'_{cb}(cbu)(1/2^+)$	6966(23)(14)	?
$\Xi^*_{cb}(cbu)(3/2^+)$	6989(24)(14)	?
$\Omega_{cb}(cbs)(1/2^+)$	6994(15)(13)	?
$\Omega'_{cb}(cbs)(1/2^+)$	7045(16)(13)	?
$\Omega^*_{cb}(cbs)(3/2^+)$	7056(17)(13)	?
$\Omega_{ccb}(1/2^+)$	8005(6)(11)	?
$\Omega^*_{ccb}(3/2^+)$	8026(7)(11)	?
$\Omega_{cbb}(1/2^+)$	11194(5)(12)	?
$\Omega^*_{cbb}(3/2^+)$	11211(6)(12)	?

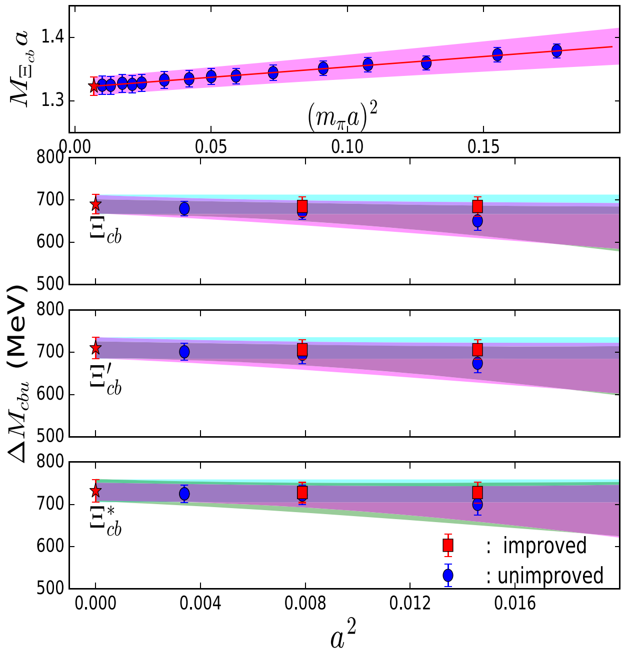

FIG. 3. (Top) Ξ_{cb} masses as a function of m_π^2. Chiral extrapolation is performed with a linear term in m_π^2. (Bottom three) Chiral extrapolated (as shown above) subtracted masses [as defined in Eq. (1)] of Ξ_{cb}, Ξ'_{cb}, and Ξ^*_{cb} baryons at three lattice spacings and at the continuum limit.

Discretization.—The adaptation of overlap fermions ensures no $\mathcal{O}(ma)$ error for light to charm quarks. The values of ma for charm quarks (0.528, 0.427, and 0.290 on three lattices) are rather small compared to unity and hence imply a smaller error from higher orders in ma. The utilization of energy splittings and ratios also ensures reduced systematics. This is clearly reflected in our estimates [66] for quarkonia hyperfine splittings [$\Delta E^{1S,\bar{c}c}_{\rm hfs} = 115(2)(3)$ MeV and $\Delta E^{1S,\bar{b}b}_{\rm hfs} = 63(3)(3)$ MeV]. These splittings are known to be quite susceptible to this error, and an excellent agreement between our and experimental values assures good control over discretization and, hence, a reliable estimation of masses of other heavy hadrons. Different fitting methods, quadratic and cubic in lattice spacing as well as both together in constrained fits, help to access possible discretization effects in continuum extrapolations. The largest discretization error is found to be for Ξ_{cb} baryons, which is about 6–7 MeV.

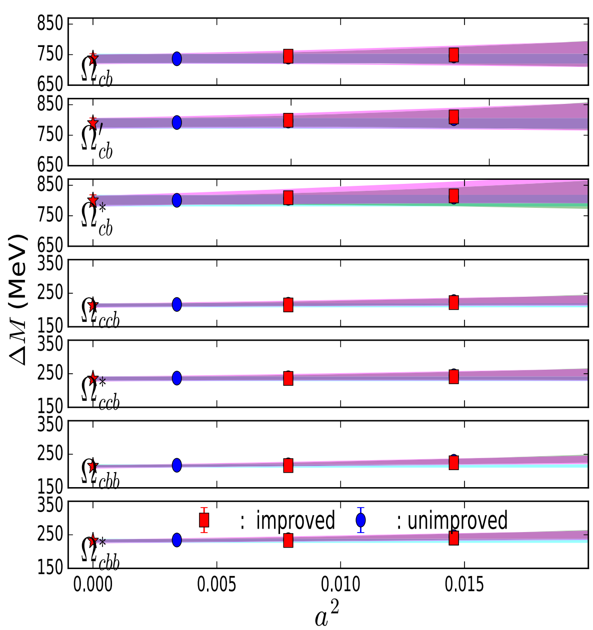

FIG. 4. Subtracted masses, as defined in Eq. (1), of Ω_{cb}, Ω'_{cb}, Ω^*_{cb} (top three), Ω_{ccb}, Ω^*_{ccb} (middle two), and Ω_{cbb}, Ω^*_{cbb} (bottom two) baryons at three lattice spacings and at the continuum limit.

Scale setting.—We independently calculated lattice spacings from Ω_{sss} baryon mass and found those to be consistent with the values measured by the MILC Collaboration [59]. The largest errors in mass splittings due this scale uncertainty are within 6 MeV.

Finite size.—The lattice volumes in this study is about 3 fm. Furthermore, the hadrons considered are quite heavy and are mostly stable to strong decays (there is no negative parity baryons). Ξ_{cb} baryons, only hadrons with valence light quark content, are found to have a perfect quadratic light quark mass dependence even towards the chiral limit, indicating no observable finite size effects in them. Conservatively, we include a maximum uncertainty of a few MeV due to finite size effects, as estimated in Ref. [57] on a similar lattice volume.

Chiral extrapolation.—In this study, only Ξ_{cb} baryons are subjected to this error. Because of the use of a multimass algorithm, we could calculate these baryons at a large number of pion masses, as shown in Fig. 3, which helps to perform extrapolations to the physical limit in a controlled and reliable way. Our results are found to be quite robust with respect to different chiral extrapolation forms.

NRQCD errors.—Since we have included terms up to $\alpha_s v^4$, higher-order terms, such as spin-dependent as well as spin-independent terms ($\alpha_s^2 v^4$ and $\alpha_s v^6$), will contribute to the systematics. For bc mesons, these errors are 4 MeV as estimated in Ref. [54] on similar lattices. As in Ref. [57], we also estimate these errors to be 5, 5, and 6 MeV for bcq, bcc, and bbc baryons, respectively.

Other errors.—Errors due to quark mass tuning are expected to be negligible in these results, considering the precision and rigor that enter into the heavy quark mass tuning procedure. The use of a wall source efficiently damps out excited state contamination, providing a long plateau in the effective mass at sufficiently large times indicating very good ground state saturation. Hence, any related uncertainties in our calculation are also negligible in comparison with any other errors. In a previous study, we also found the mixed action effects, which would vanish at the continuum limit, to be small [73] within this lattice

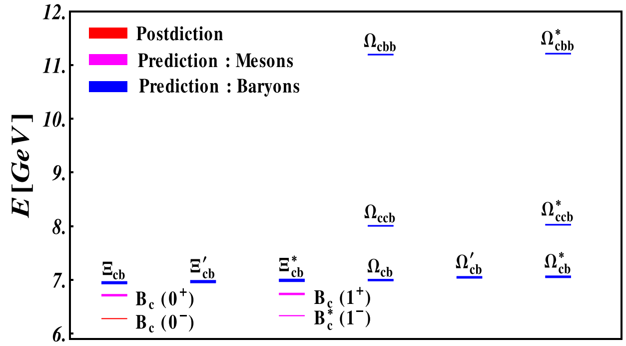

FIG. 5. Ground state masses of all bc baryons as predicted in this work.

setup. As discussed in Refs. [54,71,74] for similar lattices, the effect due to unphysical sea quark masses could be less than a percent level. Other errors due to electromagnetism, isospin breaking, and the absence of dynamical bottom quarks are expected to be within 2–4 MeV [54].

As examples, following are the systematic error budget (in MeV) for $(B_c(0^-), \Omega_{cbb})$: discretization (3, 5), scale setting (2, 6), NRQCD errors (4, 7), finite volume (0, 2), and other sources (3, 5), which when are added in quadrature lead to systematic errors as $\sim(6, 12)$ MeV.

Summary.—In this Letter, we present precise predictions of the ground state masses of bc hadrons using lattice QCD simulations with very good control over systematics. These hadrons have not been discovered yet, and, considering the recent interest in them, particularly for their relevance to the physics beyond the Standard Model, these predictions provide important information for their future discovery. Our results are based on three different lattice spacings, the finest one being 0.0582 Fermi, which help us to obtain precise results at the continuum limit. The overlap fermions, which have no $\mathcal{O}(ma)$ errors, are used for the light and strange as well as for the charm quarks. For the bottom quark, we use a nonrelativistic formulation with nonperturbatively tuned coefficients with terms up to $\mathcal{O}(\alpha_s v^4)$. The utilization of a wall source helps to extract these masses unambiguously, keeping the statistical error below the percent level. The use of mass differences as well as ratios, in which the extent of discretization effects is significantly lesser for the continuum extrapolation, enables us to predict the masses precisely. We have also addressed other possible systematic errors in detail, which when added in quadrature are found to be smaller than the statistical error in most cases. Our final results for the ground state masses of all bc hadrons are tabulated in Table II and also shown in Fig. 5.

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*nilmani@theory.tifr.res.in
†Padmanath.M@physik.uni-regensburg.de

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